

CB	LYS	A	2	5.613	-3.324	2.834	1.00	59.14	6
C	LYS	A	2	6.322	-2.753	4.050	1.00	61.37	6
C	LYS	A	2	5.431	-1.783	4.810	1.00	63.79	6
CE	LYS	A	2	5.988	-0.370	4.758	1.00	65.75	6
NZ	LYS	A	2	6.107	0.235	6.114	1.00	67.05	7
C	LYS	A	2	7.506	-2.721	1.297	1.00	54.28	6
O	LYS	A	2	8.092	-3.798	1.180	1.00	55.04	8
N	LYS	A	2	5.283	-3.329	0.369	1.00	55.75	7
CA	LYS	A	2	5.997	-2.678	1.505	1.00	55.55	6
N	ARG	A	3	8.133	-1.550	1.248	1.00	51.95	7
CA	ARG	A	3	9.568	-1.460	1.019	1.00	49.09	6
CB	ARG	A	3	9.832	-0.701	-0.286	1.00	45.74	6
C	ARG	A	3	9.634	-1.551	-1.531	1.00	42.70	6
C	ARG	A	3	9.283	-0.696	-2.736	1.00	39.77	6
N	ARG	A	3	10.401	0.132	-3.168	1.00	37.67	7
CZ	ARG	A	3	11.302	-0.211	-4.077	1.00	38.43	6
N	ARG	A	3	11.252	-1.395	-4.674	1.00	36.91	7
N	ARG	A	3	12.270	0.640	-4.395	1.00	39.50	7
C	ARG	A	3	10.314	-0.795	2.167	1.00	47.74	6
O	ARG	A	3	10.086	0.368	2.498	1.00	48.18	8
N	ARG	A	4	11.236	-1.548	2.759	1.00	45.69	7
CA	ARG	A	4	12.030	-1.079	3.884	1.00	43.14	6
CB	ARG	A	4	12.459	-2.265	4.753	1.00	45.59	6
C	ARG	A	4	11.299	-3.046	5.351	1.00	49.39	6

CA	LEU	A	1	27.715	7.796	5.976	1.00	30.88	6
CB	LEU	A	1	27.832	7.470	7.465	1.00	30.95	6
C	LEU	A	1	26.817	6.517	8.091	1.00	31.61	6
C	LEU	A	1	27.194	6.187	9.528	1.00	32.70	6
C	LEU	A	1	25.410	7.097	8.027	1.00	30.96	6
C	LEU	A	1	28.867	8.701	5.557	1.00	30.32	6
O	LEU	A	1	29.922	8.221	5.142	1.00	31.20	8
N	GLY	A	1	28.660	10.006	5.668	1.00	29.75	7
CA	GLY	A	1	29.701	10.970	5.306	1.00	29.27	6
C	GLY	A	1	29.422	12.296	6.007	1.00	28.70	6
O	GLY	A	1	28.260	12.602	6.284	1.00	28.60	8
N	MET	A	1	30.471	13.052	6.317	1.00	28.95	7
CA	MET	A	1	30.279	14.332	6.974	1.00	28.89	6
CB	MET	A	1	29.500	14.156	8.282	1.00	31.91	6
C	MET	A	1	30.318	14.051	9.554	1.00	34.60	6
SD	MET	A	1	29.290	14.107	11.033	1.00	35.65	1
CE	MET	A	1	29.116	12.360	11.381	1.00	37.75	6
C	MET	A	1	31.547	15.130	7.258	1.00	28.38	6
O	MET	A	1	32.668	14.671	7.402	1.00	27.81	8
N	LEU	A	1	31.299	16.426	7.387	1.00	27.53	7
CA	LEU	A	1	32.257	17.446	7.762	1.00	27.49	6
CB	LEU	A	1	32.577	18.409	6.630	1.00	29.94	6
C	LEU	A	1	33.334	17.830	5.431	1.00	32.91	6
C	LEU	A	1	33.043	18.630	4.173	1.00	33.46	6

**FIG. 1-1A**

C	ARG	A	4	11.719	-4.453	5.750	1.00	52.07	6
N	ARG	A	4	12.975	-4.463	6.482	1.00	56.09	7
CZ	ARG	A	4	13.402	-5.394	7.320	1.00	57.45	6
N	ARG	A	4	12.671	-6.469	7.583	1.00	58.72	7
N	ARG	A	4	14.583	-5.250	7.911	1.00	58.03	7
C	ARG	A	4	13.258	-0.297	3.435	1.00	40.93	6
O	ARG	A	4	13.873	-0.605	2.416	1.00	40.28	8
N	VAL	A	5	13.590	0.744	4.194	1.00	38.82	7
CA	VAL	A	5	14.729	1.598	3.891	1.00	37.38	6
CB	VAL	A	5	14.346	3.087	3.796	1.00	36.10	6
C	VAL	A	5	15.533	3.916	3.320	1.00	33.72	6
C	VAL	A	5	13.154	3.308	2.877	1.00	36.27	6
C	VAL	A	5	15.816	1.453	4.953	1.00	36.82	6
O	VAL	A	5	15.549	1.542	6.151	1.00	36.76	8
N	VAL	A	6	17.046	1.229	4.506	1.00	36.09	7
CA	VAL	A	6	18.188	1.076	5.394	1.00	35.35	6
C	LEU	A	1	34.828	17.784	5.721	1.00	33.17	6
C	LEU	A	1	31.597	18.185	8.933	1.00	27.03	6
O	LEU	A	1	30.438	18.586	8.823	1.00	26.86	8
N	SER	A	1	32.312	18.320	10.034	1.00	27.31	7
CA	SER	A	1	31.761	18.998	11.205	1.00	28.03	6
CB	SER	A	1	31.153	17.968	12.155	1.00	28.80	6
O	SER	A	1	32.095	17.519	13.112	1.00	31.76	8
C	SER	A	1	32.860	19.787	11.895	1.00	28.55	6
O	SER	A	1	34.043	19.612	11.612	1.00	28.57	8
N	PRO	A	1	32.488	20.594	12.880	1.00	29.49	7
C	PRO	A	1	31.084	20.865	13.288	1.00	29.61	6
CA	PRO	A	1	33.426	21.371	13.665	1.00	29.78	6
CB	PRO	A	1	32.547	22.264	14.535	1.00	29.65	6
C	PRO	A	1	31.201	22.240	13.902	1.00	29.56	6
C	PRO	A	1	34.379	20.543	14.509	1.00	30.22	6
O	PRO	A	1	35.409	21.090	14.924	1.00	30.34	8

**FIG. 1-1B**

[illegible]

**FIG. 1-1C**

C	THR	A	1	34.289	12.077	9.743	1.00	29.04	6
O	THR	A	1	34.219	12.625	10.840	1.00	28.85	8
N	VAL	A	2	33.567	11.013	9.417	1.00	29.52	7
CA	VAL	A	2	32.555	10.474	10.309	1.00	30.11	6
CB	VAL	A	2	31.750	9.352	9.621	1.00	28.43	6
C	VAL	A	2	30.737	8.721	10.564	1.00	26.35	6
C	VAL	A	2	31.036	9.898	8.392	1.00	27.62	6
C	VAL	A	2	33.145	9.945	11.609	1.00	31.80	6
O	VAL	A	2	32.732	10.364	12.694	1.00	33.28	8
N	GLU	A	2	34.091	9.018	11.517	1.00	32.42	7
CA	GLU	A	2	34.703	8.414	12.692	1.00	32.57	6
CB	GLU	A	2	35.592	7.234	12.281	1.00	34.30	6
C	GLU	A	2	34.850	6.105	11.590	1.00	36.61	6
C	GLU	A	2	33.863	5.361	12.464	1.00	39.00	6
O	GLU	A	2	33.912	5.510	13.703	1.00	40.93	8
O	GLU	A	2	33.025	4.607	11.919	1.00	39.19	8
C	GLU	A	2	35.463	9.390	13.571	1.00	32.34	6
O	GLU	A	2	35.245	9.391	14.789	1.00	33.10	8
N	SER	A	2	36.257	10.293	13.005	1.00	32.05	7
CA	SER	A	2	36.967	11.289	13.805	1.00	31.37	6
CB	SER	A	2	37.958	12.083	12.967	1.00	31.88	6
O	SER	A	2	37.334	12.786	11.911	1.00	33.76	8

C	LEU	A	2	30.408	15.892	19.038	1.00	32.71	6
C	LEU	A	2	31.823	12.851	21.736	1.00	35.01	6
O	LEU	A	2	31.378	13.316	22.788	1.00	35.64	8
N	LEU	A	2	32.280	11.605	21.655	1.00	35.18	7
CA	LEU	A	2	32.268	10.706	22.804	1.00	35.06	6
CB	LEU	A	2	32.555	9.268	22.371	1.00	32.51	6
C	LEU	A	2	31.525	8.585	21.467	1.00	29.72	6
C	LEU	A	2	31.961	7.165	21.133	1.00	26.45	6
C	LEU	A	2	30.142	8.573	22.099	1.00	26.27	6
C	LEU	A	2	33.238	11.148	23.891	1.00	35.21	6
O	LEU	A	2	32.966	10.952	25.078	1.00	36.74	8
N	ALA	A	2	34.305	11.857	23.540	1.00	34.68	7
CA	ALA	A	2	35.256	12.404	24.490	1.00	34.38	6
CB	ALA	A	2	36.650	12.454	23.870	1.00	33.09	6
C	ALA	A	2	34.873	13.794	24.980	1.00	34.57	6
O	ALA	A	2	35.624	14.411	25.741	1.00	35.34	8
N	GLY	A	3	33.741	14.327	24.544	1.00	34.34	7
CA	GLY	A	3	33.263	15.629	24.953	1.00	34.46	6
C	GLY	A	3	34.078	16.803	24.446	1.00	34.66	6
O	GLY	A	3	34.082	17.863	25.078	1.00	34.44	8
N	GLN	A	3	34.706	16.668	23.283	1.00	35.27	7
CA	GLN	A	3	35.474	17.757	22.699	1.00	36.10	6

**FIG. 1-2A**



C	SER	A	2	35.977	12.193	14.529	1.00	31.48	6
O	SER	A	2	36.173	12.531	15.698	1.00	31.98	8
N	THR	A	2	34.896	12.578	13.854	1.00	30.90	7
CA	THR	A	2	33.856	13.404	14.459	1.00	29.81	6
CB	THR	A	2	32.767	13.788	13.444	1.00	24.78	6
O	THR	A	2	33.249	14.853	12.614	1.00	25.56	8
C	THR	A	2	31.476	14.246	14.101	1.00	21.14	6
C	THR	A	2	33.215	12.612	15.601	1.00	30.00	6
O	THR	A	2	32.971	13.147	16.681	1.00	30.39	8
N	TRP	A	2	32.902	11.346	15.337	1.00	30.23	7
CA	TRP	A	2	32.277	10.472	16.324	1.00	31.17	6
CB	TRP	A	2	31.999	9.093	15.721	1.00	29.55	6
C	TRP	A	2	31.238	8.158	16.610	1.00	28.53	6
C	TRP	A	2	30.034	8.432	17.335	1.00	27.77	6
CE	TRP	A	2	29.687	7.260	18.035	1.00	27.44	6
CE	TRP	A	2	29.215	9.558	17.462	1.00	27.56	6
C	TRP	A	2	31.562	6.861	16.892	1.00	28.80	6
N	TRP	A	2	30.635	6.314	17.746	1.00	27.92	7
CZ	TRP	A	2	28.560	7.180	18.849	1.00	27.07	6
CZ	TRP	A	2	28.096	9.478	18.269	1.00	26.86	6

**FIG. 1-2B**

C	TRP	A	2	27.776	8.295	18.952	1.00	27.23	6
C	TRP	A	2	33.115	10.362	17.592	1.00	31.45	6
O	TRP	A	2	32.600	10.554	18.694	1.00	30.70	8
N	LYS	A	2	34.404	10.082	17.456	1.00	32.86	7
CA	LYS	A	2	35.321	9.952	18.576	1.00	34.03	6
CB	LYS	A	2	36.713	9.523	18.097	1.00	39.21	6
C	LYS	A	2	36.744	8.185	17.377	1.00	44.28	6
C	LYS	A	2	38.175	7.756	17.083	1.00	48.38	6
CE	LYS	A	2	38.218	6.354	16.497	1.00	50.26	6
NZ	LYS	A	2	39.243	5.508	17.170	1.00	53.04	7
C	LYS	A	2	35.456	11.231	19.393	1.00	33.60	6
O	LYS	A	2	35.500	11.178	20.626	1.00	33.43	8
N	ALA	A	2	35.493	12.381	18.727	1.00	32.92	7
CA	ALA	A	2	35.574	13.661	19.422	1.00	33.42	6
CB	ALA	A	2	35.802	14.794	18.433	1.00	32.19	6
C	ALA	A	2	34.331	13.912	20.267	1.00	33.95	6
O	ALA	A	2	34.435	14.413	21.390	1.00	34.63	8
N	LEU	A	2	33.159	13.541	19.765	1.00	34.18	7
CA	LEU	A	2	31.909	13.718	20.487	1.00	34.55	6
CB	LEU	A	2	30.710	13.432	19.585	1.00	33.95	6
C	LEU	A	2	30.303	14.460	18.534	1.00	34.29	6
C	LEU	A	2	28.879	14.174	18.065	1.00	34.02	6
C	ILE	A	3	32.210	27.780	19.950	1.00	34.80	6
C	ILE	A	3	31.583	25.307	19.990	1.00	36.07	6
C	ILE	A	3	30.154	25.663	20.253	1.00	39.29	6
C	ILE	A	3	34.994	26.875	19.184	1.00	37.54	6
O	ILE	A	3	35.710	26.788	20.180	1.00	37.10	8
N	SER	A	3	35.253	27.735	18.204	1.00	38.80	7
CA	SER	A	3	36.422	28.593	18.154	1.00	39.48	6
CB	SER	A	3	37.337	28.135	17.008	1.00	42.02	6
O	SER	A	3	38.329	27.235	17.454	1.00	46.40	8
C	SER	A	3	36.059	30.053	17.896	1.00	39.54	6
O	SER	A	3	34.918	30.363	17.558	1.00	39.54	8
N	LEU	A	3	37.045	30.937	18.011	1.00	39.16	7
CA	LEU	A	3	36.849	32.355	17.731	1.00	38.94	6
CB	LEU	A	3	37.937	33.204	18.383	1.00	41.98	6
C	LEU	A	3	37.834	33.497	19.878	1.00	43.75	6
C	LEU	A	3	39.104	34.179	20.370	1.00	44.67	6
C	LEU	A	3	36.618	34.356	20.193	1.00	44.78	6
C	LEU	A	3	36.876	32.580	16.219	1.00	38.03	6
O	LEU	A	3	37.683	31.949	15.534	1.00	38.07	8
N	ILE	A	3	36.013	33.447	15.704	1.00	37.29	7
CA	ILE	A	3	35.993	33.709	14.264	1.00	36.95	6
CB	ILE	A	3	34.716	34.443	13.832	1.00	35.68	6

FIG. 1-2C

C	ILE	A	3	34.806	34.938	12.395	1.00	34.35	6
C	ILE	A	3	33.494	33.531	13.991	1.00	36.19	6
C	ILE	A	3	32.184	34.280	14.122	1.00	36.40	6
C	ILE	A	3	37.223	34.525	13.874	1.00	37.25	6
O	ILE	A	3	37.552	35.503	14.546	1.00	36.69	8
N	ASP	A	3	37.870	34.153	12.772	1.00	38.29	7
CA	ASP	A	3	39.056	34.874	12.331	1.00	39.13	6
CB	ASP	A	3	40.318	34.057	12.629	1.00	43.72	6
C	ASP	A	3	40.275	32.654	12.064	1.00	47.45	6
O	ASP	A	3	41.077	32.344	11.160	1.00	49.13	8
O	ASP	A	3	39.444	31.842	12.525	1.00	52.02	8
C	ASP	A	3	39.025	35.267	10.863	1.00	38.42	6
O	ASP	A	3	39.957	35.946	10.414	1.00	38.79	8
N	HIS	A	3	37.971	34.930	10.127	1.00	37.59	7
CA	HIS	A	3	37.943	35.229	8.696	1.00	37.01	6
CB	HIS	A	3	37.379	34.059	7.893	1.00	36.86	6
C	HIS	A	3	36.020	33.624	8.342	1.00	37.26	6
C	HIS	A	3	35.624	32.848	9.377	1.00	37.41	6
N	HIS	A	3	34.875	34.016	7.684	1.00	37.20	7
CE	HIS	A	3	33.830	33.492	8.295	1.00	37.69	6
N	HIS	A	3	34.252	32.781	9.324	1.00	38.35	7

C	TYR	A	4	30.900	41.793	13.731	1.00	34.32	6
CE	TYR	A	4	30.682	42.017	12.383	1.00	34.43	6
C	TYR	A	4	29.040	40.311	13.795	1.00	34.03	6
CE	TYR	A	4	28.815	40.526	12.449	1.00	33.57	6
CZ	TYR	A	4	29.640	41.376	11.747	1.00	33.72	6
O	TYR	A	4	29.419	41.594	10.407	1.00	33.46	8
C	TYR	A	4	29.708	41.468	18.261	1.00	35.53	6
O	TYR	A	4	30.648	41.428	19.049	1.00	35.26	8
N	ALA	A	4	28.470	41.112	18.607	1.00	35.46	7
CA	ALA	A	4	28.129	40.652	19.946	1.00	34.81	6
CB	ALA	A	4	26.634	40.786	20.186	1.00	36.41	6
C	ALA	A	4	28.579	39.208	20.146	1.00	34.10	6
O	ALA	A	4	28.883	38.792	21.263	1.00	34.60	8
N	THR	A	4	28.586	38.435	19.067	1.00	32.65	7
CA	THR	A	4	29.063	37.056	19.106	1.00	31.17	6
CB	THR	A	4	27.988	36.038	18.717	1.00	29.80	6
O	THR	A	4	26.858	36.202	19.587	1.00	29.18	8
C	THR	A	4	28.527	34.620	18.850	1.00	26.37	6
C	THR	A	4	30.286	36.962	18.197	1.00	31.21	6
O	THR	A	4	30.245	37.331	17.024	1.00	31.46	8
N	LYS	A	4	31.396	36.508	18.768	1.00	31.20	7

**FIG. 1-3A**

C	HIS	A	3	37.241	36.534	8.359	1.00	36.69	6
O	HIS	A	3	37.175	36.922	7.190	1.00	37.23	8
N	PHE	A	4	36.755	37.250	9.362	1.00	35.95	7
CA	PHE	A	4	36.197	38.584	9.192	1.00	35.56	6
CB	PHE	A	4	34.794	38.632	8.633	1.00	31.76	6
C	PHE	A	4	33.678	38.069	9.458	1.00	31.43	6
C	PHE	A	4	33.244	36.770	9.253	1.00	27.02	6
C	PHE	A	4	33.035	38.840	10.416	1.00	28.56	6
CE	PHE	A	4	32.212	36.241	10.000	1.00	28.21	6
CE	PHE	A	4	31.998	38.315	11.163	1.00	29.67	6
CZ	PHE	A	4	31.585	37.014	10.957	1.00	27.52	6
C	PHE	A	4	36.327	39.324	10.527	1.00	36.35	6
O	PHE	A	4	36.487	38.691	11.571	1.00	35.69	8
N	ASP	A	4	36.400	40.648	10.472	1.00	37.94	7
CA	ASP	A	4	36.552	41.437	11.690	1.00	39.82	6
CB	ASP	A	4	36.910	42.886	11.349	1.00	45.32	6
C	ASP	A	4	37.632	43.576	12.491	1.00	49.18	6
O	ASP	A	4	38.498	42.932	13.121	1.00	53.55	8
O	ASP	A	4	37.336	44.758	12.759	1.00	51.63	8
C	ASP	A	4	35.290	41.390	12.541	1.00	39.52	6

**FIG. 1-3B**

[illegible]

**FIG. 1-3C**

N	LYS	A	5	37.449	23.043	10.349	1.00	36.41	7
CA	LYS	A	5	38.878	23.314	10.391	1.00	38.50	6
CB	LYS	A	5	39.363	23.117	11.840	1.00	38.42	6
C	LYS	A	5	38.814	24.167	12.794	1.00	40.28	6
C	LYS	A	5	38.770	23.668	14.228	1.00	42.84	6
CE	LYS	A	5	37.350	23.437	14.705	1.00	43.44	6
NZ	LYS	A	5	36.653	24.697	15.081	1.00	44.14	7
C	LYS	A	5	39.718	22.478	9.444	1.00	40.42	6
O	LYS	A	5	39.596	21.260	9.337	1.00	40.62	8
N	ASP	A	5	40.664	23.147	8.783	1.00	42.10	7
CA	ASP	A	5	41.617	22.514	7.881	1.00	43.84	6
CB	ASP	A	5	42.512	21.555	8.678	1.00	47.61	6
C	ASP	A	5	43.289	22.268	9.771	1.00	50.56	6
O	ASP	A	5	43.952	23.279	9.459	1.00	52.38	8
O	ASP	A	5	43.187	21.836	10.940	1.00	52.15	8
C	ASP	A	5	40.941	21.788	6.727	1.00	44.21	6
O	ASP	A	5	41.227	20.626	6.428	1.00	44.58	8
N	PHE	A	5	40.050	22.488	6.037	1.00	43.94	7
CA	PHE	A	5	39.275	21.914	4.945	1.00	44.27	6
CB	PHE	A	5	37.963	22.698	4.825	1.00	38.90	6
C	PHE	A	5	37.060	22.308	3.696	1.00	34.96	6
C	PHE	A	5	36.432	21.075	3.672	1.00	32.24	6

C	ILE	A	6	37.567	13.998	-2.774	1.00	54.63	6
C	ILE	A	6	37.223	17.225	-6.020	1.00	55.26	6
O	ILE	A	6	36.583	16.871	-7.013	1.00	54.72	8
N	ILE	A	6	37.389	18.509	-5.720	1.00	55.58	7
CA	ILE	A	6	36.959	19.594	-6.587	1.00	56.21	6
CB	ILE	A	6	35.885	20.502	-5.963	1.00	54.72	6
C	ILE	A	6	35.379	21.516	-6.985	1.00	53.62	6
C	ILE	A	6	34.697	19.717	-5.404	1.00	54.25	6
C	ILE	A	6	34.399	20.027	-3.952	1.00	53.74	6
C	ILE	A	6	38.151	20.477	-6.962	1.00	57.36	6
O	ILE	A	6	38.886	20.940	-6.089	1.00	56.79	8
N	SER	A	6	38.297	20.751	-8.254	1.00	59.16	7
CA	SER	A	6	39.409	21.565	-8.732	1.00	61.00	6
CB	SER	A	6	39.496	21.520	-10.258	1.00	61.46	6
O	SER	A	6	38.215	21.648	-10.849	1.00	63.02	8
C	SER	A	6	39.286	23.007	-8.261	1.00	62.26	6
O	SER	A	6	38.203	23.459	-7.890	1.00	62.61	8
N	ARG	A	6	40.389	23.749	-8.340	1.00	63.24	7
CA	ARG	A	6	40.391	25.163	-7.975	1.00	64.33	6
CB	ARG	A	6	41.798	25.733	-7.862	1.00	70.36	6
C	ARG	A	6	42.847	24.781	-7.312	1.00	75.55	6
C	ARG	A	6	43.965	24.570	-8.322	1.00	79.64	6

**FIG. 1-4A**

C	PHE	A	5	36.827	23.193	2.653	1.00	33.21	6
CE	PHE	A	5	35.597	20.725	2.629	1.00	31.61	6
CE	PHE	A	5	35.992	22.848	1.607	1.00	32.75	6
CZ	PHE	A	5	35.377	21.612	1.595	1.00	32.24	6
C	PHE	A	5	40.028	21.868	3.627	1.00	45.76	6
O	PHE	A	5	40.511	22.875	3.115	1.00	45.77	8
N	ASN	A	5	40.109	20.672	3.051	1.00	47.93	7
CA	ASN	A	5	40.764	20.458	1.769	1.00	50.19	6
CB	ASN	A	5	42.108	19.750	1.930	1.00	55.16	6
C	ASN	A	5	42.893	19.657	0.637	1.00	59.33	6
O	ASN	A	5	43.373	18.585	0.266	1.00	61.85	8
N	ASN	A	5	43.038	20.776	-0.065	1.00	60.64	7
C	ASN	A	5	39.860	19.647	0.842	1.00	50.97	6
O	ASN	A	5	39.380	18.573	1.203	1.00	51.24	8
N	CYS	A	5	39.606	20.198	-0.338	1.00	51.32	7
CA	CYS	A	5	38.762	19.529	-1.322	1.00	52.14	6
CB	CYS	A	5	37.365	20.144	-1.347	1.00	52.43	6
SG	CYS	A	5	37.309	21.830	-1.997	1.00	50.96	1
C	CYS	A	5	39.408	19.600	-2.699	1.00	52.89	6

**FIG. 1-4B**





C	ARG	A	6	33.541	29.463	-8.272	1.00	42.38	6
O	ARG	A	6	32.974	30.555	-8.163	1.00	42.43	8
N	LYS	A	6	32.895	28.387	-8.698	1.00	38.98	7
CA	LYS	A	6	31.489	28.391	-9.047	1.00	36.08	6
CB	LYS	A	6	31.233	27.425	-10.211	1.00	38.25	6
C	LYS	A	6	32.187	27.547	-11.385	1.00	41.26	6
C	LYS	A	6	31.832	26.533	-12.467	1.00	43.21	6
CE	LYS	A	6	32.688	26.729	-13.707	1.00	45.12	6
NZ	LYS	A	6	32.841	25.473	-14.491	1.00	44.54	7
C	LYS	A	6	30.595	27.970	-7.885	1.00	33.41	6
O	LYS	A	6	29.393	27.786	-8.094	1.00	32.34	8
N	MET	A	7	31.148	27.782	-6.690	1.00	31.31	7
CA	MET	A	7	30.352	27.276	-5.584	1.00	30.21	6
CB	MET	A	7	30.475	25.744	-5.527	1.00	32.32	6
C	MET	A	7	31.857	25.194	-5.822	1.00	35.12	6
SD	MET	A	7	31.957	23.402	-5.704	1.00	36.02	1
CE	MET	A	7	31.529	22.901	-7.367	1.00	34.53	6
C	MET	A	7	30.684	27.848	-4.215	1.00	28.31	6
O	MET	A	7	31.832	27.922	-3.787	1.00	28.11	8
N	ASP	A	7	29.624	28.234	-3.503	1.00	25.95	7
CA	ASP	A	7	29.766	28.751	-2.143	1.00	23.65	6
C	TVR	A	7	30.779	23.481	5.163	1.00	25.10	6
CE	TYR	A	7	31.538	24.408	5.853	1.00	25.02	6
C	TYR	A	7	32.615	23.038	3.717	1.00	25.66	6
CE	TVR	A	7	33.382	23.970	4.390	1.00	25.67	6
CZ	TYR	A	7	32.835	24.651	5.457	1.00	25.21	6
O	TYR	A	7	33.592	25.576	6.133	1.00	25.47	8
C	TVR	A	7	30.106	19.904	1.768	1.00	23.62	6
O	TYR	A	7	30.406	18.741	2.037	1.00	23.40	8
N	GLY	A	7	28.986	20.218	1.124	1.00	22.96	7
CA	GLY	A	7	28.018	19.230	0.696	1.00	23.75	6
C	GLY	A	7	28.588	18.158	-0.218	1.00	24.27	6
O	GLY	A	7	28.290	16.977	-0.034	1.00	23.78	8
N	ILE	A	7	29.369	18.551	-1.219	1.00	25.10	7
CA	ILE	A	7	29.975	17.602	-2.144	1.00	25.73	6
CB	ILE	A	7	30.674	18.315	-3.316	1.00	27.05	6
C	ILE	A	7	31.383	17.316	-4.222	1.00	27.14	6
C	ILE	A	7	29.645	19.119	-4.117	1.00	27.25	6
C	ILE	A	7	30.230	20.052	-5.152	1.00	29.01	6
C	ILE	A	7	30.945	16.669	-1.430	1.00	25.57	6
O	ILE	A	7	30.797	15.447	-1.504	1.00	24.87	8
N	VAL	A	7	31.896	17.231	-0.691	1.00	25.62	7

**FIG. 1-5A**

[illegible]

**FIG. 1-5B**



O	MET	A	8	29.873	5.147	-1.919	1.00	37.28	8
N	GLN	A	8	31.338	6.765	-1.397	1.00	37.87	7
CA	GLN	A	8	32.462	5.860	-1.192	1.00	38.47	6
CB	GLN	A	8	33.741	6.661	-0.925	1.00	39.65	6
C	GLN	A	8	34.320	7.292	-2.182	1.00	41.26	6
C	GLN	A	8	35.553	8.126	-1.924	1.00	44.46	6
O	GLN	A	8	35.965	8.328	-0.781	1.00	48.85	8
N	GLN	A	8	36.170	8.625	-2.991	1.00	45.09	7
C	GLN	A	8	32.195	4.862	-0.077	1.00	38.33	6
O	GLN	A	8	32.309	3.653	-0.293	1.00	38.79	8
N	ASP	A	8	31.705	5.316	1.071	1.00	38.25	7
CA	ASP	A	8	31.356	4.431	2.171	1.00	38.61	6
CB	ASP	A	8	30.800	5.221	3.364	1.00	35.92	6
C	ASP	A	8	30.769	4.381	4.627	1.00	34.86	6
O	ASP	A	8	31.730	3.609	4.836	1.00	38.15	8
O	ASP	A	8	29.807	4.473	5.413	1.00	32.47	8
C	ASP	A	8	30.338	3.362	1.785	1.00	39.15	6
O	ASP	A	8	30.418	2.228	2.261	1.00	39.15	8
N	SER	A	8	29.341	3.717	0.987	1.00	40.00	7
CA	SER	A	8	28.268	2.824	0.605	1.00	40.96	6
CB	SER	A	8	27.186	3.609	-0.151	1.00	37.71	6
O	SER	A	8	27.641	3.995	-1.435	1.00	34.05	8
C	GLU	A	9	23.353	4.138	-20.431	1.00	70.30	6
O	GLU	A	9	22.552	5.077	-20.630	1.00	70.81	8
O	GLU	A	9	24.484	4.092	-20.959	1.00	72.24	8
C	GLU	A	9	22.261	2.275	-16.722	1.00	60.55	6
O	GLU	A	9	21.246	2.969	-16.829	1.00	60.93	8
N	GLU	A	9	22.187	1.025	-16.283	1.00	60.08	7
CA	GLU	A	9	20.972	0.362	-15.864	1.00	59.62	6
CB	GLU	A	9	21.143	-1.161	-15.975	1.00	65.14	6
C	GLU	A	9	20.576	-1.748	-17.254	1.00	70.30	6
C	GLU	A	9	21.426	-2.860	-17.834	1.00	73.39	6
O	GLU	A	9	21.214	-4.032	-17.458	1.00	74.84	8
O	GLU	A	9	22.302	-2.564	-18.674	1.00	74.99	8
C	GLU	A	9	20.570	0.709	-14.432	1.00	57.78	6
O	GLU	A	9	19.505	0.300	-13.964	1.00	58.25	8
N	ASN	A	9	21.403	1.442	-13.708	1.00	55.25	7
CA	ASN	A	9	21.154	1.857	-12.345	1.00	52.48	6
CB	ASN	A	9	22.436	1.692	-11.509	1.00	52.33	6
C	ASN	A	9	22.256	0.836	-10.279	1.00	52.34	6
O	ASN	A	9	21.147	0.414	-9.952	1.00	53.95	8
N	ASN	A	9	23.355	0.564	-9.584	1.00	52.48	7
C	ASN	A	9	20.747	3.320	-12.209	1.00	50.29	6
O	ASN	A	9	19.918	3.684	-11.376	1.00	49.91	8

**FIG. 1-6A**



[illegible]

**FIG. 1-6C**

CB	ALA	A	1	16.330	13.994	-0.604	1.00	20.94	6
C	ALA	A	1	18.266	15.578	-0.290	1.00	23.06	6
O	ALA	A	1	18.438	15.176	0.858	1.00	22.58	8
N	ILE	A	1	18.951	16.600	-0.799	1.00	22.65	7
CA	ILE	A	1	19.890	17.384	-0.008	1.00	22.42	6
CB	ILE	A	1	21.308	17.361	-0.609	1.00	19.84	6
C	ILE	A	1	22.263	18.211	0.218	1.00	19.61	6
C	ILE	A	1	21.846	15.931	-0.727	1.00	19.04	6
C	ILE	A	1	22.912	15.769	-1.789	1.00	14.64	6
C	ILE	A	1	19.430	18.837	0.103	1.00	22.33	6
O	ILE	A	1	19.185	19.485	-0.912	1.00	22.91	8
N	GLY	A	1	19.398	19.363	1.321	1.00	21.49	7
CA	GLY	A	1	18.983	20.732	1.546	1.00	21.32	6
C	GLY	A	1	19.985	21.571	2.326	1.00	21.77	6
O	GLY	A	1	21.116	21.201	2.619	1.00	20.74	8
N	SER	A	1	19.526	22.767	2.663	1.00	22.27	7
CA	SER	A	1	20.263	23.779	3.400	1.00	22.50	6
CB	SER	A	1	21.306	24.448	2.511	1.00	22.72	6
O	SER	A	1	22.078	25.395	3.224	1.00	21.91	8
C	SER	A	1	19.248	24.811	3.895	1.00	22.77	6
O	SER	A	1	18.261	25.058	3.198	1.00	22.73	8

C	ILE	A	1	23.320	37.452	-1.351	1.00	20.68	6
C	ILE	A	1	23.558	35.053	-2.019	1.00	21.17	6
C	ILE	A	1	22.467	34.395	-1.206	1.00	20.81	6
C	ILE	A	1	26.148	37.861	-1.461	1.00	22.38	6
O	ILE	A	1	25.969	38.896	-2.103	1.00	21.79	8
N	GLU	A	1	26.848	37.829	-0.332	1.00	22.40	7
CA	GLU	A	1	27.490	39.019	0.209	1.00	23.90	6
CB	GLU	A	1	28.076	38.737	1.590	1.00	23.43	6
C	GLU	A	1	27.029	38.487	2.666	1.00	24.28	6
C	GLU	A	1	27.682	38.221	4.010	1.00	26.12	6
O	GLU	A	1	27.217	37.322	4.736	1.00	24.90	8
O	GLU	A	1	28.671	38.918	4.318	1.00	28.72	8
C	GLU	A	1	28.575	39.538	-0.727	1.00	24.96	6
O	GLU	A	1	28.586	40.724	-1.050	1.00	25.66	8
N	GLU	A	1	29.464	38.665	-1.189	1.00	26.22	7
CA	GLU	A	1	30.525	39.052	-2.107	1.00	27.40	6
CB	GLU	A	1	31.361	37.838	-2.520	1.00	29.69	6
C	GLU	A	1	32.500	38.186	-3.466	1.00	36.82	6
C	GLU	A	1	33.298	36.974	-3.901	1.00	39.85	6
O	GLU	A	1	34.033	36.420	-3.058	1.00	42.55	8
O	GLU	A	1	33.191	36.575	-5.079	1.00	43.21	8

**FIG. 1-7A**

N	GLY	A	1	19.473	25.393	5.062	1.00	22.84	7
CA	GLY	A	1	18.557	26.368	5.619	1.00	23.14	6
C	GLY	A	1	18.683	27.762	5.036	1.00	23.90	6
O	GLY	A	1	17.665	28.437	4.846	1.00	23.26	8
N	I LE	A	1	19.904	28.234	4.800	1.00	24.27	7
CA	I LE	A	1	20.130	29.582	4.284	1.00	25.21	6
CB	I LE	A	1	20.904	30.424	5.317	1.00	28.84	6
C	I LE	A	1	21.399	31.746	4.750	1.00	29.40	6
C	I LE	A	1	20.025	30.718	6.544	1.00	30.94	6
C	I LE	A	1	20.804	31.053	7.796	1.00	32.04	6
C	I LE	A	1	20.839	29.580	2.938	1.00	25.28	6
O	I LE	A	1	20.712	30.527	2.153	1.00	25.17	8
N	GLY	A	1	21.587	28.527	2.623	1.00	25.28	7
CA	GLY	A	1	22.284	28.453	1.345	1.00	25.24	6
C	GLY	A	1	23.457	29.418	1.274	1.00	25.63	6
O	GLY	A	1	24.083	29.755	2.279	1.00	25.92	8
N	GLY	A	1	23.862	29.789	0.062	1.00	25.45	7
CA	GLY	A	1	25.084	30.496	-0.218	1.00	26.20	6
C	GLY	A	1	25.213	31.934	0.223	1.00	27.33	6
O	GLY	A	1	25.522	32.817	-0.585	1.00	27.71	8
N	LEU	A	1	25.181	32.186	1.526	1.00	27.58	7

**FIG. 1-7B**





CB	MET	A	1	27.435	47.984	-3.301	1.00	52.03	6
C	MET	A	1	26.067	48.225	-2.680	1.00	57.93	6
SD	MET	A	1	26.084	48.049	-0.886	1.00	64.29	1
CE	MET	A	1	26.407	49.739	-0.383	1.00	64.73	6
C	MET	A	1	28.613	49.012	-5.246	1.00	47.07	6
O	MET	A	1	28.443	50.220	-5.426	1.00	47.31	8
N	ASN	A	1	29.799	48.433	-5.396	1.00	46.74	7
CA	ASN	A	1	30.983	49.177	-5.779	1.00	46.35	6
CB	ASN	A	1	32.214	48.573	-5.088	1.00	45.88	6
C	ASN	A	1	32.174	48.660	-3.581	1.00	45.33	6
O	ASN	A	1	32.794	47.836	-2.904	1.00	46.65	8
N	ASN	A	1	31.462	49.639	-3.037	1.00	44.11	7
C	ASN	A	1	31.255	49.202	-7.277	1.00	45.75	6
O	ASN	A	1	32.177	49.917	-7.685	1.00	46.59	8
N	GLY	A	1	30.574	48.383	-8.072	1.00	44.74	7
CA	GLY	A	1	30.922	48.253	-9.474	1.00	43.33	6
C	GLY	A	1	29.781	48.197	-10.464	1.00	42.25	6
O	GLY	A	1	30.035	48.292	-11.671	1.00	42.48	8
N	GLY	A	1	28.543	48.053	-10.006	1.00	41.17	7
CA	GLY	A	1	27.409	47.945	-10.932	1.00	39.64	6
C	GLY	A	1	27.225	46.464	-11.262	1.00	38.72	6

C	PRO	A	1	30.522	35.725	-13.712	1.00	30.70	6
CA	PRO	A	1	28.262	34.851	-13.934	1.00	30.42	6
CB	PRO	A	1	29.075	34.511	-15.176	1.00	30.53	6
C	PRO	A	1	30.497	34.659	-14.773	1.00	30.46	6
C	PRO	A	1	27.747	33.598	-13.247	1.00	29.81	6
O	PRO	A	1	26.717	33.040	-13.634	1.00	30.42	8
N	PHE	A	1	28.418	33.122	-12.205	1.00	29.31	7
CA	PHE	A	1	27.966	31.998	-11.409	1.00	28.57	6
CB	PHE	A	1	29.165	31.134	-10.994	1.00	32.50	6
C	PHE	A	1	30.000	30.707	-12.171	1.00	35.29	6
C	PHE	A	1	31.285	31.197	-12.336	1.00	36.91	6
C	PHE	A	1	29.496	29.828	-13.114	1.00	36.02	6
CE	PHE	A	1	32.054	30.816	-13.420	1.00	36.75	6
CE	PHE	A	1	30.259	29.444	-14.200	1.00	37.47	6
CZ	PHE	A	1	31.539	29.939	-14.352	1.00	37.10	6
C	PHE	A	1	27.152	32.407	-10.189	1.00	27.24	6
O	PHE	A	1	26.811	31.525	-9.391	1.00	26.69	8
N	PHE	A	1	26.728	33.662	-10.062	1.00	26.22	7
CA	PHE	A	1	25.921	34.075	-8.923	1.00	26.42	6
CB	PHE	A	1	25.261	35.452	-9.115	1.00	28.07	6
C	PHE	A	1	24.327	35.782	-7.976	1.00	29.48	6

**FIG. 1-8A**





CA	VAL	A	1	19.895	25.653	-2.121	1.00	25.35	6
CB	VAL	A	1	18.603	25.780	-1.273	1.00	27.33	6
C	VAL	A	1	18.095	24.469	-0.709	1.00	29.41	6
C	VAL	A	1	18.866	26.764	-0.133	1.00	28.85	6
C	VAL	A	1	19.959	24.312	-2.815	1.00	25.00	6
O	VAL	A	1	20.571	23.385	-2.257	1.00	24.69	8
N	ASN	A	1	19.368	24.140	-3.991	1.00	24.21	7
CA	ASN	A	1	19.357	22.841	-4.651	1.00	24.07	6
CB	ASN	A	1	18.105	22.748	-5.540	1.00	22.14	6
C	ASN	A	1	18.226	23.637	-6.762	1.00	22.88	6
O	ASN	A	1	18.291	24.859	-6.633	1.00	22.25	8
N	ASN	A	1	18.316	23.019	-7.933	1.00	22.17	7
C	ASN	A	1	20.613	22.517	-5.443	1.00	24.43	6
O	ASN	A	1	20.701	21.419	-6.008	1.00	23.79	8
N	MET	A	1	21.630	23.371	-5.435	1.00	25.03	7
CA	MET	A	1	22.850	23.139	-6.196	1.00	26.58	6
CB	MET	A	1	23.547	24.458	-6.529	1.00	27.98	6
C	MET	A	1	22.821	25.227	-7.629	1.00	32.05	6
SD	MET	A	1	22.346	24.205	-9.040	1.00	35.93	1
CE	MET	A	1	23.951	23.688	-9.643	1.00	36.90	6
C	MET	A	1	23.777	22.099	-5.593	1.00	27.33	6

CA	ILE	A	1	26.035	15.369	-12.394	1.00	37.59	6
CB	ILE	A	1	26.478	16.811	-12.704	1.00	38.89	6
C	ILE	A	1	27.394	16.854	-13.919	1.00	37.93	6
C	ILE	A	1	25.266	17.723	-12.924	1.00	38.70	6
C	ILE	A	1	25.565	19.186	-12.670	1.00	37.99	6
C	ILE	A	1	27.283	14.521	-12.164	1.00	37.96	6
O	ILE	A	1	27.627	13.656	-12.966	1.00	38.29	8
N	MET	A	1	27.967	14.762	-11.053	1.00	37.90	7
CA	MET	A	1	29.175	14.047	-10.686	1.00	38.24	6
CB	MET	A	1	29.616	14.468	-9.277	1.00	39.44	6
C	MET	A	1	30.324	15.813	-9.239	1.00	40.87	6
SD	MET	A	1	30.886	16.247	-7.581	1.00	42.12	1
CE	MET	A	1	32.332	15.198	-7.440	1.00	41.22	6
C	MET	A	1	29.056	12.531	-10.747	1.00	37.94	6
O	MET	A	1	29.979	11.880	-11.247	1.00	38.17	8
N	TYR	A	1	27.984	11.945	-10.223	1.00	37.10	7
CA	TYR	A	1	27.818	10.501	-10.220	1.00	36.19	6
CB	TYR	A	1	27.350	10.040	-8.822	1.00	36.32	6
C	TYR	A	1	28.508	10.115	-7.843	1.00	36.68	6
C	TYR	A	1	28.715	11.251	-7.073	1.00	36.50	6
CE	TYR	A	1	29.778	11.325	-6.193	1.00	36.74	6

**FIG. 1-9A**

O	MET	A	1	24.655	21.602	-6.317	1.00	28.18	8
N	VAL	A	1	23.598	21.699	-4.337	1.00	27.13	7
CA	VAL	A	1	24.425	20.637	-3.771	1.00	27.35	6
CB	VAL	A	1	24.341	20.475	-2.251	1.00	27.90	6
C	VAL	A	1	25.288	19.352	-1.785	1.00	25.87	6
C	VAL	A	1	24.698	21.767	-1.536	1.00	25.87	6
C	VAL	A	1	23.973	19.328	-4.435	1.00	27.41	6
O	VAL	A	1	24.783	18.507	-4.856	1.00	28.08	8
N	ALA	A	1	22.658	19.158	-4.561	1.00	27.02	7
CA	ALA	A	1	22.079	17.988	-5.214	1.00	26.49	6
CB	ALA	A	1	20.598	17.856	-4.897	1.00	21.24	6
C	ALA	A	1	22.302	18.059	-6.723	1.00	26.51	6
O	ALA	A	1	22.549	17.048	-7.378	1.00	25.54	8
N	GLY	A	1	22.291	19.270	-7.275	1.00	27.35	7
CA	GLY	A	1	22.623	19.479	-8.678	1.00	28.51	6
C	GLY	A	1	24.041	18.991	-8.970	1.00	29.26	6
O	GLY	A	1	24.238	18.218	-9.905	1.00	29.73	8
N	HIS	A	1	25.018	19.404	-8.172	1.00	30.44	7
CA	HIS	A	1	26.403	19.012	-8.362	1.00	31.50	6
CB	HIS	A	1	27.347	19.828	-7.458	1.00	31.18	6
C	HIS	A	1	27.723	21.121	-8.124	1.00	30.77	6

**FIG. 1-9B**



O	SER	A	1	18.098	16.586	-7.525	1.00	33.35	8
C	SER	A	1	15.482	16.210	-6.329	1.00	26.68	6
O	SER	A	1	14.883	17.041	-7.016	1.00	26.03	8
N	ILE	A	1	15.474	16.244	-4.995	1.00	26.03	7
CA	ILE	A	1	14.787	17.320	-4.297	1.00	25.17	6
CB	ILE	A	1	13.482	16.951	-3.579	1.00	24.96	6
C	ILE	A	1	12.331	16.776	-4.559	1.00	22.35	6
C	ILE	A	1	13.650	15.714	-2.691	1.00	22.54	6
C	ILE	A	1	12.588	15.627	-1.610	1.00	19.83	6
C	ILE	A	1	15.709	17.968	-3.259	1.00	25.23	6
O	ILE	A	1	16.762	17.455	-2.899	1.00	24.97	8
N	SER	A	1	15.272	19.131	-2.791	1.00	23.95	7
CA	SER	A	1	15.975	19.891	-1.776	1.00	23.50	6
CB	SER	A	1	16.846	20.992	-2.374	1.00	22.64	6
O	SER	A	1	17.886	20.488	-3.183	1.00	24.55	8
C	SER	A	1	14.954	20.529	-0.830	1.00	22.76	6
O	SER	A	1	14.208	21.410	-1.268	1.00	22.27	8
N	ILE	A	1	14.925	20.083	0.422	1.00	21.99	7
CA	ILE	A	1	13.988	20.677	1.379	1.00	21.74	6
CB	ILE	A	1	13.273	19.657	2.271	1.00	19.43	6
C	ILE	A	1	12.340	20.363	3.253	1.00	18.21	6

O	GLY	A	1	17.502	15.461	7.132	1.00	24.80	8
N	VAL	A	1	16.529	16.677	8.744	1.00	25.23	7
CA	VAL	A	1	15.568	15.639	9.104	1.00	26.31	6
CB	VAL	A	1	14.954	15.935	10.485	1.00	26.54	6
C	VAL	A	1	13.631	15.222	10.713	1.00	28.08	6
C	VAL	A	1	15.946	15.553	11.579	1.00	25.33	6
C	VAL	A	1	14.485	15.475	8.048	1.00	26.62	6
O	VAL	A	1	14.045	14.351	7.792	1.00	27.98	8
N	HIS	A	1	14.039	16.570	7.442	1.00	26.00	7
CA	HIS	A	1	12.999	16.512	6.424	1.00	24.82	6
CB	HIS	A	1	12.453	17.908	6.120	1.00	23.96	6
C	HIS	A	1	11.405	18.394	7.069	1.00	23.62	6
C	HIS	A	1	10.606	17.745	7.947	1.00	22.84	6
N	HIS	A	1	11.084	19.733	7.180	1.00	22.53	7
CE	HIS	A	1	10.136	19.880	8.085	1.00	21.95	6
N	HIS	A	1	9.828	18.691	8.571	1.00	22.11	7
C	HIS	A	1	13.505	15.866	5.138	1.00	24.05	6
O	HIS	A	1	12.780	15.110	4.489	1.00	23.48	8
N	ASN	A	1	14.738	16.191	4.760	1.00	23.02	7
CA	ASN	A	1	15.337	15.637	3.551	1.00	22.46	6
CB	ASN	A	1	16.657	16.341	3.249	1.00	20.13	6

**FIG. 1-10A**



C	ILE	A	1	12.485	18.680	1.394	1.00	16.47	6
C	ILE	A	1	11.801	17.553	2.125	1.00	15.87	6
C	ILE	A	1	14.732	21.721	2.212	1.00	21.86	6
O	ILE	A	1	15.832	21.490	2.710	1.00	22.41	8
N	ALA	A	1	14.136	22.904	2.305	1.00	21.42	7
CA	ALA	A	1	14.730	24.012	3.047	1.00	20.33	6
CB	ALA	A	1	15.008	25.172	2.105	1.00	16.53	6
C	ALA	A	1	13.798	24.428	4.180	1.00	19.82	6
O	ALA	A	1	12.924	25.278	4.015	1.00	18.81	8
N	THR	A	1	13.981	23.797	5.336	1.00	19.95	7
CA	THR	A	1	13.149	24.098	6.499	1.00	20.29	6
CB	THR	A	1	12.256	22.902	6.879	1.00	18.29	6
O	THR	A	1	13.009	21.692	6.725	1.00	17.31	8
C	THR	A	1	11.023	22.835	5.992	1.00	13.32	6
C	THR	A	1	14.011	24.514	7.684	1.00	20.40	6
O	THR	A	1	13.897	23.945	8.770	1.00	20.37	8
N	ALA	A	1	14.905	25.476	7.453	1.00	20.45	7
CA	ALA	A	1	15.764	25.976	8.530	1.00	21.02	6
CB	ALA	A	1	14.946	26.878	9.445	1.00	18.59	6

**FIG. 1-10B**



CZ	ARG	A	1	6.668	9.071	6.379	1.00	25.51	6
N	ARG	A	1	7.531	8.100	6.653	1.00	25.70	7
N	ARG	A	1	6.027	9.664	7.383	1.00	22.96	7
C	ARG	A	1	9.337	7.947	0.146	1.00	29.05	6
O	ARG	A	1	8.764	6.963	-0.322	1.00	28.83	8
N	ILE	A	1	10.175	8.700	-0.571	1.00	29.97	7
CA	ILE	A	1	10.412	8.435	-1.987	1.00	30.60	6
CB	ILE	A	1	11.472	9.361	-2.602	1.00	29.35	6
C	ILE	A	1	11.847	8.928	-4.014	1.00	26.83	6
C	ILE	A	1	10.983	10.815	-2.636	1.00	30.12	6
C	ILE	A	1	12.070	11.813	-2.989	1.00	30.42	6
C	ILE	A	1	10.797	6.975	-2.206	1.00	31.59	6
O	ILE	A	1	10.158	6.295	-3.013	1.00	31.73	8
N	ILE	A	1	11.810	6.481	-1.498	1.00	32.37	7
CA	ILE	A	1	12.236	5.092	-1.645	1.00	33.03	6
CB	ILE	A	1	13.463	4.776	-0.770	1.00	32.09	6
C	ILE	A	1	13.683	3.280	-0.605	1.00	32.34	6
C	ILE	A	1	14.690	5.435	-1.408	1.00	29.55	6
C	ILE	A	1	15.962	5.310	-0.614	1.00	26.75	6
C	ILE	A	1	11.111	4.111	-1.362	1.00	33.89	6
O	ILE	A	1	10.851	3.228	-2.183	1.00	34.76	8
N	ALA	A	1	10.379	4.296	-0.271	1.00	33.88	7

CA	VAL	A	1	18.917	4.578	-3.508	1.00	33.83	6
CB	VAL	A	1	20.345	4.287	-4.011	1.00	35.53	6
C	VAL	A	1	21.388	4.950	-3.114	1.00	36.35	6
C	VAL	A	1	20.639	2.798	-4.108	1.00	35.37	6
C	VAL	A	1	18.733	6.096	-3.518	1.00	33.19	6
O	VAL	A	1	18.432	6.683	-4.555	1.00	33.44	8
N	MET	A	1	18.951	6.739	-2.378	1.00	32.55	7
CA	MET	A	1	18.937	8.186	-2.263	1.00	31.13	6
CB	MET	A	1	17.660	8.727	-1.631	1.00	29.51	6
C	MET	A	1	16.342	8.551	-2.341	1.00	29.70	6
SD	MET	A	1	16.246	9.357	-3.946	1.00	29.08	1
CE	MET	A	1	15.597	10.961	-3.486	1.00	31.20	6
C	MET	A	1	20.109	8.666	-1.395	1.00	30.44	6
O	MET	A	1	20.302	8.170	-0.284	1.00	29.87	8
N	VAL	A	1	20.857	9.642	-1.890	1.00	29.52	7
CA	VAL	A	1	21.815	10.382	-1.073	1.00	28.81	6
CB	VAL	A	1	22.956	11.026	-1.865	1.00	30.53	6
C	VAL	A	1	24.149	11.320	-0.962	1.00	29.68	6
C	VAL	A	1	23.391	10.162	-3.041	1.00	32.18	6
C	VAL	A	1	21.003	11.492	-0.394	1.00	28.25	6
O	VAL	A	1	20.334	12.247	-1.103	1.00	28.36	8
N	ALA	A	1	21.009	11.563	0.927	1.00	28.00	7

**FIG. 1-11A**





CB	SER	A	1	30.187	30.978	10.425	1.00	22.54	6
O	SER	A	1	30.945	30.242	9.481	1.00	25.70	8
C	SER	A	1	29.753	32.948	8.915	1.00	23.53	6
O	SER	A	1	30.941	32.962	8.617	1.00	24.01	8
N	THR	A	1	28.929	33.890	8.475	1.00	23.83	7
CA	THR	A	1	29.327	35.046	7.696	1.00	23.35	6
CB	THR	A	1	28.751	35.080	6.270	1.00	22.12	6
O	THR	A	1	27.347	35.382	6.337	1.00	21.97	8
C	THR	A	1	28.954	33.781	5.510	1.00	16.87	6
C	THR	A	1	28.827	36.288	8.434	1.00	23.72	6
O	THR	A	1	27.950	36.195	9.293	1.00	24.19	8
N	PRO	A	1	29.316	37.457	8.053	1.00	24.41	7
C	PRO	A	1	30.360	37.644	7.012	1.00	24.34	6
CA	PRO	A	1	28.891	38.718	8.633	1.00	25.09	6
CB	PRO	A	1	29.459	39.754	7.663	1.00	25.21	6
C	PRO	A	1	30.683	39.111	7.107	1.00	24.81	6
C	PRO	A	1	27.385	38.854	8.766	1.00	26.19	6
O	PRO	A	1	26.860	39.216	9.820	1.00	26.80	8
N	LEU	A	1	26.649	38.559	7.699	1.00	26.66	7
CA	LEU	A	1	25.198	38.611	7.668	1.00	26.40	6
CB	LEU	A	1	24.707	38.491	6.223	1.00	27.52	6
C	LEU	A	1	23.511	39.326	5.775	1.00	28.54	6

O	ALA	A	2	18.132	41.553	16.760	1.00	32.29	8
N	ALA	A	2	18.560	39.424	16.211	1.00	32.49	7
CA	ALA	A	2	17.363	38.876	16.825	1.00	33.33	6
CB	ALA	A	2	16.872	37.674	16.026	1.00	31.09	6
C	ALA	A	2	17.627	38.463	18.270	1.00	33.90	6
O	ALA	A	2	16.754	37.938	18.963	1.00	33.89	8
N	ARG	A	2	18.869	38.611	18.722	1.00	34.28	7
CA	ARG	A	2	19.287	38.270	20.070	1.00	34.97	6
CB	ARG	A	2	18.524	39.123	21.090	1.00	38.59	6
C	ARG	A	2	18.886	40.600	21.079	1.00	41.47	6
C	ARG	A	2	18.409	41.314	22.337	1.00	43.64	6
N	ARG	A	2	18.620	40.498	23.526	1.00	46.60	7
CZ	ARG	A	2	17.676	40.032	24.333	1.00	46.43	6
N	ARG	A	2	18.031	39.291	25.377	1.00	45.04	7
N	ARG	A	2	16.394	40.294	24.113	1.00	45.74	7
C	ARG	A	2	19.102	36.788	20.376	1.00	34.33	6
O	ARG	A	2	18.837	36.404	21.515	1.00	35.01	8
N	ALA	A	2	19.323	35.933	19.386	1.00	33.04	7
CA	ALA	A	2	19.103	34.501	19.508	1.00	32.04	6
CB	ALA	A	2	18.494	33.973	18.211	1.00	31.13	6
C	ALA	A	2	20.396	33.748	19.798	1.00	31.06	6
O	ALA	A	2	20.383	32.573	20.149	1.00	30.34	8

**FIG. 1-12A**



O	GLY	A	2	22.738	39.970	13.505	1.00	27.08	8
N	GLY	A	2	22.838	38.762	11.627	1.00	26.23	7
CA	GLY	A	2	21.413	38.550	11.495	1.00	24.79	6
C	GLY	A	2	20.776	37.836	12.672	1.00	24.76	6
O	GLY	A	2	19.736	38.245	13.187	1.00	25.40	8
N	PHE	A	2	21.406	36.755	13.116	1.00	24.57	7
CA	PHE	A	2	20.938	35.996	14.269	1.00	24.30	6
CB	PHE	A	2	21.573	34.611	14.314	1.00	22.09	6
C	PHE	A	2	20.910	33.583	13.445	1.00	21.81	6
C	PHE	A	2	21.598	33.006	12.390	1.00	22.56	6
C	PHE	A	2	19.605	33.183	13.683	1.00	21.56	6
CE	PHE	A	2	20.998	32.056	11.585	1.00	20.56	6
CE	PHE	A	2	18.998	32.232	12.885	1.00	21.92	6
CZ	PHE	A	2	19.699	31.668	11.835	1.00	20.90	6
C	PHE	A	2	21.280	36.791	15.531	1.00	24.51	6
O	PHE	A	2	20.522	36.827	16.493	1.00	23.72	8
N	GLY	A	2	22.385	37.529	15.481	1.00	25.54	7
CA	GLY	A	2	22.787	38.466	16.513	1.00	27.69	6
C	GLY	A	2	21.755	39.569	16.716	1.00	29.46	6
O	GLY	A	2	21.429	39.940	17.845	1.00	30.10	8
N	ALA	A	2	21.197	40.082	15.625	1.00	30.15	7
CA	ALA	A	2	20.195	41.129	15.617	1.00	30.95	6
CB	ALA	A	2	19.958	41.606	14.186	1.00	31.39	6
C	ALA	A	2	18.870	40.715	16.238	1.00	32.05	6

C	THR	A	2	27.416	38.794	24.035	1.00	42.95	6
C	THR	A	2	28.441	36.006	24.708	1.00	36.70	6
O	THR	A	2	29.285	36.866	24.973	1.00	36.29	8
N	ARG	A	2	28.636	34.756	25.133	1.00	36.20	7
CA	ARG	A	2	29.705	34.383	26.051	1.00	36.03	6
CB	ARG	A	2	29.360	33.028	26.690	1.00	35.31	6
C	ARG	A	2	30.100	32.742	27.985	1.00	37.08	6
C	ARG	A	2	29.729	31.380	28.553	1.00	40.22	6
N	ARG	A	2	28.718	31.483	29.599	1.00	44.00	7
CZ	ARG	A	2	27.407	31.439	29.399	1.00	47.44	6
N	ARG	A	2	26.904	31.286	28.179	1.00	48.14	7
N	ARG	A	2	26.581	31.547	30.433	1.00	48.31	7
C	ARG	A	2	31.085	34.338	25.417	1.00	36.15	6
O	ARG	A	2	31.717	33.282	25.333	1.00	34.44	8
N	ASN	A	2	31.642	35.480	25.025	1.00	37.86	7
CA	ASN	A	2	32.943	35.576	24.394	1.00	40.94	6
CB	ASN	A	2	33.150	36.977	23.797	1.00	43.10	6
C	ASN	A	2	32.132	37.323	22.732	1.00	45.64	6
O	ASN	A	2	32.199	36.833	21.602	1.00	48.03	8
N	ASN	A	2	31.175	38.174	23.082	1.00	44.97	7
C	ASN	A	2	34.118	35.264	25.307	1.00	42.95	6
O	ASN	A	2	35.199	34.931	24.811	1.00	43.48	8
N	ASP	A	2	33.952	35.353	26.622	1.00	45.18	7
CA	ASP	A	2	35.028	35.065	27.564	1.00	47.07	6

**FIG. 1-12C**



CB	ASP	A	2	34.667	35.501	28.983	1.00	53.38	6
C	ASP	A	2	33.371	34.900	29.487	1.00	58.02	6
O	ASP	A	2	32.291	35.360	29.058	1.00	61.40	8
O	ASP	A	2	33.426	33.965	30.313	1.00	60.57	8
C	ASP	A	2	35.396	33.585	27.518	1.00	46.62	6
O	ASP	A	2	36.563	33.215	27.634	1.00	46.96	8
N	ASN	A	2	34.396	32.737	27.314	1.00	45.88	7
CA	ASN	A	2	34.589	31.298	27.205	1.00	44.67	6
CB	ASN	A	2	34.307	30.646	28.555	1.00	47.32	6
C	ASN	A	2	34.731	29.206	28.693	1.00	49.19	6
O	ASN	A	2	34.710	28.665	29.804	1.00	51.07	8
N	ASN	A	2	35.110	28.548	27.605	1.00	50.01	7
C	ASN	A	2	33.702	30.716	26.111	1.00	43.18	6
O	ASN	A	2	32.596	30.231	26.353	1.00	43.11	8
N	PRO	A	2	34.198	30.724	24.877	1.00	41.75	7
C	PRO	A	2	35.503	31.329	24.497	1.00	41.44	6
CA	PRO	A	2	33.490	30.210	23.722	1.00	40.67	6
CB	PRO	A	2	34.468	30.398	22.564	1.00	40.80	6
C	PRO	A	2	35.391	31.478	23.004	1.00	41.02	6
C	PRO	A	2	33.042	28.763	23.813	1.00	39.35	6
O	PRO	A	2	31.944	28.425	23.353	1.00	38.82	8
N	GLN	A	2	33.830	27.881	24.419	1.00	37.99	7

N	TRP	A	2	20.006	23.348	28.471	1.00	38.16	7
CA	TRP	A	2	19.340	23.015	29.712	1.00	39.63	6
CB	TRP	A	2	19.102	21.506	29.803	1.00	35.31	6
C	TRP	A	2	18.105	20.982	28.812	1.00	33.04	6
C	TRP	A	2	18.371	20.039	27.765	1.00	32.01	6
CE	TRP	A	2	17.161	19.826	27.079	1.00	31.00	6
CE	TRP	A	2	19.518	19.357	27.344	1.00	32.03	6
C	TRP	A	2	16.781	21.294	28.719	1.00	30.50	6
N	TRP	A	2	16.206	20.601	27.681	1.00	29.81	7
CZ	TRP	A	2	17.062	18.957	25.994	1.00	32.45	6
CZ	TRP	A	2	19.420	18.496	26.268	1.00	34.32	6
C	TRP	A	2	18.199	18.306	25.607	1.00	34.41	6
C	TRP	A	2	20.014	23.518	30.980	1.00	41.79	6
O	TRP	A	2	19.477	23.335	32.077	1.00	42.19	8
N	ASP	A	2	21.147	24.190	30.865	1.00	43.09	7
CA	ASP	A	2	21.818	24.835	31.980	1.00	44.52	6
CB	ASP	A	2	23.278	25.103	31.631	1.00	43.42	6
C	ASP	A	2	24.118	25.502	32.825	1.00	43.46	6
O	ASP	A	2	24.475	26.697	32.926	1.00	42.68	8
O	ASP	A	2	24.445	24.622	33.647	1.00	42.29	8
C	ASP	A	2	21.084	26.137	32.293	1.00	45.89	6
O	ASP	A	2	20.438	26.712	31.414	1.00	46.28	8

FIG. 1-13A

CA	GLN	A	2	33.509	26.472	24.546	1.00	36.26	6
CB	GLN	A	2	34.772	25.643	24.816	1.00	39.69	6
C	GLN	A	2	35.799	25.668	23.704	1.00	44.96	6
C	GLN	A	2	37.042	26.454	24.073	1.00	48.84	6
O	GLN	A	2	36.960	27.544	24.642	1.00	49.73	8
N	GLN	A	2	38.202	25.894	23.745	1.00	51.41	7
C	GLN	A	2	32.499	26.138	25.635	1.00	34.32	6
O	GLN	A	2	32.096	24.976	25.739	1.00	32.80	8
N	ALA	A	2	32.114	27.094	26.466	1.00	33.94	7
CA	ALA	A	2	31.137	26.852	27.521	1.00	33.57	6
CB	ALA	A	2	31.693	27.300	28.865	1.00	32.53	6
C	ALA	A	2	29.837	27.588	27.213	1.00	33.31	6
O	ALA	A	2	28.850	27.491	27.940	1.00	33.64	8
N	ALA	A	2	29.847	28.327	26.111	1.00	32.94	7
CA	ALA	A	2	28.700	29.104	25.669	1.00	32.57	6
CB	ALA	A	2	29.084	29.939	24.455	1.00	33.89	6
C	ALA	A	2	27.498	28.226	25.350	1.00	32.18	6
O	ALA	A	2	26.384	28.515	25.790	1.00	32.83	8
N	SER	A	2	27.716	27.171	24.574	1.00	31.80	7
CA	SER	A	2	26.628	26.259	24.222	1.00	31.73	6
CB	SER	A	2	26.971	25.487	22.951	1.00	30.83	6
O	SER	A	2	25.928	24.593	22.607	1.00	29.99	8

N	LYS	A	2	21.191	26.613	33.526	1.00	46.55	7
CA	LYS	A	2	20.516	27.826	33.956	1.00	46.61	6
CB	LYS	A	2	20.543	27.916	35.490	1.00	49.39	6
C	LYS	A	2	21.936	28.097	36.070	1.00	51.89	6
C	LYS	A	2	21.944	29.115	37.199	1.00	54.74	6
CE	LYS	A	2	22.163	30.525	36.679	1.00	56.43	6
NZ	LYS	A	2	23.250	31.225	37.419	1.00	57.67	7
C	LYS	A	2	21.084	29.104	33.361	1.00	46.01	6
O	LYS	A	2	20.356	30.093	33.235	1.00	45.69	8
N	GLU	A	2	22.357	29.115	32.989	1.00	45.88	7
CA	GLU	A	2	23.003	30.286	32.424	1.00	45.19	6
CB	GLU	A	2	24.486	30.296	32.810	1.00	49.81	6
C	GLU	A	2	24.786	30.476	34.291	1.00	55.39	6
C	GLU	A	2	26.292	30.404	34.508	1.00	58.82	6
O	GLU	A	2	26.965	31.416	34.221	1.00	61.25	8
O	GLU	A	2	26.780	29.338	34.934	1.00	61.03	8
C	GLU	A	2	22.903	30.411	30.910	1.00	43.34	6
O	GLU	A	2	23.571	31.282	30.338	1.00	43.47	8
N	ARG	A	2	22.109	29.591	30.240	1.00	41.68	7
CA	ARG	A	2	21.890	29.686	28.809	1.00	39.75	6
CB	ARG	A	2	20.645	28.904	28.382	1.00	39.29	6
C	ARG	A	2	20.740	27.401	28.338	1.00	38.54	6

**FIG. 1-13B**



CA	PHE	A	2	22.371	29.067	20.587	1.00	25.74	6
CB	PHE	A	2	21.471	28.412	19.546	1.00	25.79	6
C	PHE	A	2	21.216	29.119	18.254	1.00	24.95	6
C	PHE	A	2	22.114	29.029	17.203	1.00	24.19	6
C	PHE	A	2	20.068	29.876	18.077	1.00	23.27	6
CE	PHE	A	2	21.878	29.680	16.007	1.00	25.52	6
CE	PHE	A	2	19.825	30.531	16.884	1.00	24.37	6
CZ	PHE	A	2	20.731	30.434	15.848	1.00	25.52	6
C	PHE	A	2	23.710	29.499	20.011	1.00	23.85	6
O	PHE	A	2	24.058	30.676	19.954	1.00	22.69	8
N	VAL	A	2	24.512	28.501	19.649	1.00	23.40	7
CA	VAL	A	2	25.827	28.727	19.061	1.00	23.14	6
CB	VAL	A	2	26.963	28.060	19.845	1.00	21.81	6
C	VAL	A	2	28.308	28.317	19.177	1.00	21.07	6
C	VAL	A	2	27.009	28.565	21.282	1.00	26.15	6
C	VAL	A	2	25.815	28.227	17.615	1.00	22.86	6
O	VAL	A	2	25.369	27.121	17.331	1.00	21.50	8
N	LEU	A	2	26.245	29.082	16.701	1.00	23.86	7
CA	LEU	A	2	26.240	28.798	15.274	1.00	25.13	6
CB	LEU	A	2	26.346	30.119	14.519	1.00	29.61	6
C	LEU	A	2	25.871	30.274	13.085	1.00	33.44	6
C	LEU	A	2	24.777	29.293	12.696	1.00	35.45	6
C	LEU	A	2	25.382	31.707	12.865	1.00	34.21	6
C	LEU	A	2	27.377	27.868	14.868	1.00	25.05	6

C	LEU	A	2	23.205	8.789	2.973	1.00	31.47	6
O	LEU	A	2	22.504	9.447	2.213	1.00	32.20	8
N	VAL	A	2	23.559	7.529	2.753	1.00	31.86	7
CA	VAL	A	2	23.031	6.776	1.629	1.00	32.03	6
CB	VAL	A	2	24.033	5.825	0.970	1.00	31.99	6
C	VAL	A	2	23.378	5.082	-0.190	1.00	33.53	6
C	VAL	A	2	25.261	6.577	0.485	1.00	31.64	6
C	VAL	A	2	21.851	5.964	2.178	1.00	32.37	6
O	VAL	A	2	22.003	5.194	3.124	1.00	32.10	8
N	LEU	A	2	20.675	6.234	1.633	1.00	32.90	7
CA	LEU	A	2	19.473	5.506	2.023	1.00	32.91	6
CB	LEU	A	2	18.307	6.453	2.270	1.00	32.52	6
C	LEU	A	2	18.303	7.271	3.561	1.00	31.91	6
C	LEU	A	2	17.139	8.254	3.566	1.00	32.20	6
C	LEU	A	2	18.230	6.365	4.779	1.00	33.24	6
C	LEU	A	2	19.146	4.547	0.882	1.00	33.63	6
O	LEU	A	2	19.229	4.984	-0.271	1.00	33.36	8
N	GLU	A	2	18.806	3.297	1.169	1.00	35.24	7
CA	GLU	A	2	18.428	2.403	0.074	1.00	37.02	6
CB	GLU	A	2	19.635	1.854	-0.663	1.00	39.18	6
C	GLU	A	2	20.444	0.775	0.026	1.00	41.57	6
C	GLU	A	2	21.610	0.335	-0.845	1.00	43.33	6
O	GLU	A	2	22.733	0.832	-0.631	1.00	42.15	8
O	GLU	A	2	21.393	-0.501	-1.748	1.00	46.02	8

**FIG. 1-14A**

**FIG. 1-14B**

**FIG. 1-14B**



C	HIS	A	2	19.852	-3.972	-2.410	1.00	47.38	6
O	HIS	A	2	20.841	-4.346	-3.035	1.00	47.01	8
N	ALA	A	2	19.918	-3.568	-1.146	1.00	49.48	7
CA	ALA	A	2	21.156	-3.512	-0.387	1.00	51.58	6
CB	ALA	A	2	20.957	-2.642	0.850	1.00	50.94	6
C	ALA	A	2	21.672	-4.883	0.025	1.00	53.16	6
O	ALA	A	2	22.872	-5.150	-0.033	1.00	53.00	8
N	LYS	A	2	20.762	-5.756	0.439	1.00	55.23	7
CA	LYS	A	2	21.119	-7.119	0.829	1.00	57.65	6
CB	LYS	A	2	19.908	-7.816	1.441	1.00	60.63	6
C	LYS	A	2	20.032	-9.315	1.639	1.00	65.05	6
C	LYS	A	2	18.678	-9.947	1.929	1.00	67.78	6
CE	LYS	A	2	18.832	-	2.540	1.00	69.75	6
NZ	LYS	A	2	17.937	-	3.715	1.00	71.19	7
C	LYS	A	2	21.651	-7.883	-0.379	1.00	58.57	6
O	LYS	A	2	22.648	-8.601	-0.295	1.00	59.09	8
N	LYS	A	2	21.013	-7.719	-1.532	1.00	59.06	7
CA	LYS	A	2	21.396	-8.367	-2.775	1.00	59.54	6
CB	LYS	A	2	20.417	-7.977	-3.889	1.00	61.74	6
C	LYS	A	2	20.739	-8.548	-5.257	1.00	64.55	6
C	LYS	A	2	19.526	-8.538	-6.174	1.00	67.02	6
CE	LYS	A	2	18.684	-9.790	-5.989	1.00	67.96	6
NZ	LYS	A	2	17.562	-9.562	-5.037	1.00	69.74	7
C	LYS	A	2	22.823	-8.063	-3.209	1.00	59.47	6
O	LYS	A	2	23.481	-8.928	-3.797	1.00	59.77	8

CB	TYR	A	2	24.564	2.118	9.276	1.00	36.36	6
C	TYR	A	2	25.973	2.410	8.826	1.00	33.88	6
C	TYR	A	2	26.265	2.576	7.480	1.00	33.29	6
CE	TYR	A	2	27.553	2.850	7.058	1.00	33.19	6
C	TYR	A	2	27.007	2.532	9.744	1.00	32.95	6
CE	TYR	A	2	28.298	2.805	9.331	1.00	32.34	6
CZ	TYR	A	2	28.562	2.963	7.990	1.00	32.93	6
O	TYR	A	2	29.843	3.235	7.572	1.00	33.91	8
C	TYR	A	2	23.010	0.588	10.393	1.00	37.77	6
O	TYR	A	2	23.112	0.610	11.619	1.00	37.81	8
N	ALA	A	2	21.839	0.629	9.769	1.00	37.28	7
CA	ALA	A	2	20.581	0.637	10.500	1.00	36.62	6
CB	ALA	A	2	20.556	1.758	11.528	1.00	37.87	6
C	ALA	A	2	19.407	0.791	9.536	1.00	36.09	6
O	ALA	A	2	19.578	0.861	8.320	1.00	35.78	8
N	GLU	A	2	18.214	0.845	10.109	1.00	35.82	7
CA	GLU	A	2	16.988	0.971	9.338	1.00	35.66	6
CB	GLU	A	2	16.120	-0.270	9.577	1.00	37.13	6
C	GLU	A	2	14.914	-0.407	8.670	1.00	40.33	6
C	GLU	A	2	14.032	-1.593	8.998	1.00	41.53	6
O	GLU	A	2	12.858	-1.611	8.569	1.00	42.20	8
O	GLU	A	2	14.495	-2.527	9.684	1.00	44.11	8
C	GLU	A	2	16.206	2.219	9.719	1.00	35.25	6
O	GLU	A	2	16.047	2.517	10.903	1.00	35.55	8
N	LEU	A	2	15.720	2.940	8.714	1.00	35.26	7

**FIG. 1-15A**







C	MET	A	2	5.090	16.631	11.707	1.00	29.62	6
O	MET	A	2	3.994	16.089	11.829	1.00	29.55	8
N	SER	A	2	5.320	17.892	12.046	1.00	29.54	7
CA	SER	A	2	4.278	18.725	12.629	1.00	29.53	6
CB	SER	A	2	4.122	18.390	14.119	1.00	30.34	6
O	SER	A	2	5.115	19.081	14.866	1.00	29.32	8
C	SER	A	2	4.615	20.207	12.499	1.00	29.31	6
O	SER	A	2	5.715	20.579	12.098	1.00	28.62	8
N	SER	A	2	3.671	21.054	12.890	1.00	29.86	7
CA	SER	A	2	3.872	22.489	12.941	1.00	30.22	6
CB	SER	A	2	3.231	23.285	11.817	1.00	27.32	6
O	SER	A	2	3.053	22.555	10.628	1.00	25.45	8
C	SER	A	2	3.324	22.997	14.282	1.00	31.35	6
O	SER	A	2	2.380	22.420	14.814	1.00	32.24	8
N	ASP	A	2	3.914	24.073	14.780	1.00	31.85	7
CA	ASP	A	2	3.515	24.660	16.043	1.00	32.92	6
CB	ASP	A	2	4.679	25.459	16.645	1.00	28.71	6
C	ASP	A	2	5.764	24.604	17.259	1.00	25.31	6
O	ASP	A	2	5.563	23.380	17.390	1.00	23.22	8
O	ASP	A	2	6.818	25.182	17.601	1.00	20.63	8
C	ASP	A	2	2.342	25.623	15.912	1.00	34.31	6
O	ASP	A	2	1.535	25.753	16.831	1.00	35.57	8
N	ALA	A	2	2.280	26.342	14.796	1.00	35.24	7
CA	ALA	A	2	1.222	27.322	14.562	1.00	35.86	6

N	SER	A	2	9.879	31.662	18.196	1.00	46.47	7
CA	SER	A	2	9.714	31.026	19.495	1.00	47.43	6
CB	SER	A	2	9.270	32.058	20.538	1.00	49.71	6
O	SER	A	2	10.284	33.013	20.790	1.00	52.26	8
C	SER	A	2	8.701	29.888	19.459	1.00	47.25	6
O	SER	A	2	7.660	29.962	18.811	1.00	47.41	8
N	PRO	A	2	8.982	28.840	20.221	1.00	46.81	7
C	PRO	A	2	10.212	28.661	21.033	1.00	46.92	6
CA	PRO	A	2	8.101	27.693	20.357	1.00	46.66	6
CB	PRO	A	2	9.087	26.562	20.623	1.00	46.56	6
C	PRO	A	2	10.210	27.194	21.365	1.00	46.64	6
C	PRO	A	2	7.137	27.868	21.518	1.00	46.77	6
O	PRO	A	2	7.342	28.716	22.390	1.00	46.67	8
N	PRO	A	2	6.072	27.078	21.539	1.00	47.01	7
C	PRO	A	2	5.770	26.011	20.560	1.00	46.89	6
CA	PRO	A	2	5.129	27.090	22.643	1.00	47.40	6
CB	PRO	A	2	3.973	26.227	22.173	1.00	47.06	6
C	PRO	A	2	4.400	25.537	20.935	1.00	47.05	6
C	PRO	A	2	5.789	26.528	23.889	1.00	47.82	6
O	PRO	A	2	6.397	25.453	23.831	1.00	47.54	8
N	GLU	A	2	5.619	27.172	25.038	1.00	48.53	7
CA	GLU	A	2	6.188	26.696	26.299	1.00	49.69	6
CB	GLU	A	2	5.816	27.643	27.441	1.00	55.27	6
C	GLU	A	2	6.199	29.094	27.188	1.00	61.22	6

**FIG. 1-16A**

[illegible]

**FIG. 1-16B**



C	LEU	A	2	0.415	18.015	16.133	1.00	40.11	6
C	LEU	A	2	0.639	15.522	16.125	1.00	41.11	6
C	LEU	A	2	4.007	15.066	16.966	1.00	34.13	6
O	LEU	A	2	3.695	13.968	16.499	1.00	33.81	8
N	ALA	A	2	5.152	15.667	16.648	1.00	33.82	7
CA	ALA	A	2	6.119	15.068	15.736	1.00	33.23	6
CB	ALA	A	2	7.212	16.070	15.395	1.00	32.79	6
C	ALA	A	2	6.713	13.783	16.305	1.00	32.82	6
O	ALA	A	2	6.930	12.826	15.555	1.00	31.82	8
N	MET	A	2	6.969	13.751	17.614	1.00	32.44	7
CA	MET	A	2	7.455	12.516	18.239	1.00	32.54	6
CB	MET	A	2	7.999	12.771	19.636	1.00	32.06	6
C	MET	A	2	9.285	13.590	19.637	1.00	30.75	6
SD	MET	A	2	10.047	13.718	21.262	1.00	31.85	1
CE	MET	A	2	9.278	15.202	21.899	1.00	24.03	6
C	MET	A	2	6.317	11.502	18.214	1.00	32.99	6
O	MET	A	2	6.464	10.387	17.711	1.00	33.07	8
N	ALA	A	2	5.123	11.934	18.613	1.00	33.83	7
CA	ALA	A	2	3.931	11.100	18.540	1.00	34.86	6
CB	ALA	A	2	2.696	11.897	18.938	1.00	36.22	6
C	ALA	A	2	3.739	10.514	17.145	1.00	35.40	6
O	ALA	A	2	3.541	9.302	17.030	1.00	36.47	8
N	ASN	A	2	3.817	11.328	16.094	1.00	35.07	7
CA	ASN	A	2	3.628	10.851	14.733	1.00	34.90	6

CB	ALA	A	2	8.334	3.400	14.135	1.00	42.87	6
C	ALA	A	2	6.335	1.908	13.964	1.00	42.62	6
O	ALA	A	2	6.650	0.731	13.796	1.00	43.14	8
N	GLY	A	2	5.304	2.271	14.719	1.00	43.20	7
CA	GLY	A	2	4.452	1.297	15.387	1.00	43.62	6
C	GLY	A	2	5.114	0.739	16.638	1.00	43.92	6
O	GLY	A	2	5.107	-0.466	16.884	1.00	44.21	8
N	ILE	A	2	5.771	1.613	17.390	1.00	43.72	7
CA	ILE	A	2	6.425	1.245	18.635	1.00	43.55	6
CB	ILE	A	2	7.958	1.199	18.545	1.00	42.75	6
C	ILE	A	2	8.444	-0.071	17.859	1.00	41.52	6
C	ILE	A	2	8.506	2.431	17.820	1.00	42.54	6
C	ILE	A	2	9.940	2.759	18.178	1.00	43.11	6
C	ILE	A	2	6.023	2.261	19.704	1.00	43.86	6
O	ILE	A	2	5.637	3.378	19.357	1.00	43.43	8
N	GLU	A	2	6.097	1.867	20.968	1.00	45.03	7
CA	GLU	A	2	5.758	2.805	22.040	1.00	46.66	6
CB	GLU	A	2	5.132	2.074	23.223	1.00	53.41	6
C	GLU	A	2	3.772	1.466	22.905	1.00	60.11	6
C	GLU	A	2	2.955	1.176	24.149	1.00	64.17	6
O	GLU	A	2	2.576	0.003	24.354	1.00	66.12	8
O	GLU	A	2	2.690	2.121	24.922	1.00	66.54	8
C	GLU	A	2	7.005	3.582	22.436	1.00	46.19	6
O	GLU	A	2	8.121	3.206	22.071	1.00	45.77	8

**FIG. 1-17A**



[illegible]

**FIG. 1-17C**

CZ	TYR	A	2	21.905	10.777	21.621	1.00	35.72	6
O	TYR	A	2	22.617	11.885	21.218	1.00	35.48	8
C	TYR	A	2	17.576	8.447	22.237	1.00	36.52	6
O	TYR	A	2	17.242	8.145	21.096	1.00	35.93	8
N	VAL	A	3	17.430	9.680	22.716	1.00	35.99	7
CA	VAL	A	3	16.887	10.788	21.955	1.00	35.60	6
CB	VAL	A	3	15.694	11.455	22.668	1.00	37.52	6
C	VAL	A	3	15.134	12.606	21.839	1.00	38.08	6
C	VAL	A	3	14.592	10.451	22.970	1.00	39.63	6
C	VAL	A	3	17.958	11.856	21.725	1.00	34.43	6
O	VAL	A	3	18.409	12.496	22.675	1.00	33.82	8
N	ASN	A	3	18.389	12.018	20.480	1.00	34.00	7
CA	ASN	A	3	19.251	13.152	20.122	1.00	32.94	6
CB	ASN	A	3	19.999	12.918	18.828	1.00	33.36	6
C	ASN	A	3	21.046	13.957	18.499	1.00	35.05	6
O	ASN	A	3	22.239	13.747	18.730	1.00	36.83	8
N	ASN	A	3	20.620	15.086	17.946	1.00	35.26	7
C	ASN	A	3	18.307	14.355	20.032	1.00	32.21	6
O	ASN	A	3	17.477	14.448	19.130	1.00	31.53	8
N	ALA	A	3	18.392	15.219	21.029	1.00	31.54	7
CA	ALA	A	3	17.516	16.366	21.148	1.00	31.65	6
CB	ALA	A	3	17.630	16.910	22.576	1.00	27.55	6
C	ALA	A	3	17.819	17.498	20.183	1.00	31.57	6

O	PRO	A	3	14.346	27.732	27.366	1.00	39.90	8
N	ALA	A	3	13.863	29.551	26.149	1.00	38.58	7
CA	ALA	A	3	12.543	29.093	25.745	1.00	38.47	6
CB	ALA	A	3	11.890	30.148	24.855	1.00	38.42	6
C	ALA	A	3	12.517	27.741	25.053	1.00	38.11	6
O	ALA	A	3	11.657	26.908	25.367	1.00	38.32	8
N	GLY	A	3	13.404	27.502	24.096	1.00	37.82	7
CA	GLY	A	3	13.418	26.268	23.333	1.00	37.36	6
C	GLY	A	3	13.765	25.021	24.125	1.00	37.41	6
O	GLY	A	3	13.141	23.971	23.945	1.00	36.65	8
N	ASP	A	3	14.746	25.106	25.018	1.00	38.18	7
CA	ASP	A	3	15.180	23.961	25.811	1.00	39.15	6
CB	ASP	A	3	16.465	24.288	26.575	1.00	40.44	6
C	ASP	A	3	17.674	24.427	25.673	1.00	41.01	6
O	ASP	A	3	18.777	24.687	26.198	1.00	41.45	8
O	ASP	A	3	17.544	24.277	24.441	1.00	42.11	8
C	ASP	A	3	14.107	23.470	26.771	1.00	39.31	6
O	ASP	A	3	13.965	22.262	26.962	1.00	38.78	8
N	LYS	A	3	13.337	24.384	27.349	1.00	40.33	7
CA	LYS	A	3	12.248	24.038	28.249	1.00	41.37	6
CB	LYS	A	3	11.679	25.294	28.915	1.00	44.75	6
C	LYS	A	3	12.447	25.786	30.127	1.00	48.79	6
C	LYS	A	3	11.955	27.158	30.569	1.00	52.90	6

**FIG. 1-18A**



O	ALA	A	3	18.915	17.585	19.637	1.00	31.93	8
N	HIS	A	3	16.837	18.396	20.037	1.00	31.47	7
CA	HIS	A	3	17.066	19.582	19.205	1.00	31.50	6
CB	HIS	A	3	15.774	20.293	18.825	1.00	30.71	6
C	HIS	A	3	16.012	21.492	17.954	1.00	30.47	6
C	HIS	A	3	16.639	21.604	16.758	1.00	30.33	6
N	HIS	A	3	15.623	22.765	18.306	1.00	31.27	7
CE	HIS	A	3	15.990	23.610	17.361	1.00	31.78	6
N	HIS	A	3	16.610	22.932	16.411	1.00	32.01	7
C	HIS	A	3	18.023	20.467	20.012	1.00	31.54	6
O	HIS	A	3	19.076	20.889	19.544	1.00	31.65	8
N	GLY	A	3	17.751	20.594	21.304	1.00	31.96	7
CA	GLY	A	3	18.569	21.240	22.298	1.00	32.18	6
C	GLY	A	3	19.554	22.282	21.817	1.00	32.16	6
O	GLY	A	3	20.765	22.041	21.787	1.00	32.53	8
N	THR	A	3	19.075	23.478	21.485	1.00	32.26	7
CA	THR	A	3	19.942	24.526	20.965	1.00	30.30	6
CB	THR	A	3	19.195	25.393	19.926	1.00	31.30	6
O	THR	A	3	17.971	25.868	20.489	1.00	33.79	8

**FIG. 1-18B**



C	VAL	A	3	11.856	14.898	25.087	1.00	46.70	6
C	VAL	A	3	8.919	13.883	27.364	1.00	47.82	6
O	VAL	A	3	8.604	12.693	27.365	1.00	47.71	8
N	LVS	A	3	8.585	14.714	28.349	1.00	48.07	7
CA	LVS	A	3	7.799	14.263	29.494	1.00	48.68	6
CB	LVS	A	3	7.654	15.386	30.523	1.00	48.79	6
C	LVS	A	3	8.880	15.539	31.412	1.00	49.95	6
C	LVS	A	3	8.716	16.660	32.425	1.00	51.90	6
CE	LVS	A	3	9.831	16.618	33.459	1.00	53.93	6
NZ	LVS	A	3	9.808	17.806	34.357	1.00	55.89	7
C	LVS	A	3	6.439	13.762	29.024	1.00	49.02	6
O	LVS	A	3	6.044	12.632	29.302	1.00	49.46	8
N	THR	A	3	5.771	14.551	28.192	1.00	48.90	7
CA	THR	A	3	4.469	14.237	27.636	1.00	49.03	6
CB	THR	A	3	3.972	15.427	26.782	1.00	48.10	6
O	THR	A	3	4.097	16.635	27.549	1.00	47.21	8
C	THR	A	3	2.522	15.250	26.372	1.00	46.85	6
C	THR	A	3	4.411	12.968	26.804	1.00	49.57	6
O	THR	A	3	3.380	12.285	26.804	1.00	50.05	8
N	ILE	A	3	5.462	12.637	26.068	1.00	50.18	7
CA	ILE	A	3	5.470	11.469	25.198	1.00	50.51	6

O	SER	A	3	12.171	8.052	35.359	1.00	57.76	8
C	SER	A	3	14.399	7.821	33.107	1.00	56.08	6
O	SER	A	3	15.603	7.733	33.355	1.00	56.24	8
N	ARG	A	3	13.781	6.902	32.386	1.00	56.22	7
CA	ARG	A	3	14.416	5.726	31.814	1.00	56.26	6
CB	ARG	A	3	13.344	4.651	31.647	1.00	61.19	6
C	ARG	A	3	13.701	3.372	30.920	1.00	66.66	6
C	ARG	A	3	12.447	2.526	30.737	1.00	71.39	6
N	ARG	A	3	12.695	1.230	30.126	1.00	75.06	7
CZ	ARG	A	3	11.756	0.312	29.913	1.00	77.16	6
N	ARG	A	3	10.497	0.540	30.262	1.00	78.29	7
N	ARG	A	3	12.073	-0.845	29.347	1.00	78.92	7
C	ARG	A	3	15.110	6.023	30.491	1.00	55.03	6
O	ARG	A	3	16.028	5.296	30.105	1.00	55.13	8
N	VAL	A	3	14.705	7.077	29.789	1.00	53.57	7
CA	VAL	A	3	15.284	7.424	28.496	1.00	51.50	6
CB	VAL	A	3	14.174	7.860	27.515	1.00	51.84	6
C	VAL	A	3	13.523	9.165	27.947	1.00	51.31	6
C	VAL	A	3	14.710	7.972	26.095	1.00	51.08	6
C	VAL	A	3	16.377	8.479	28.545	1.00	49.96	6
O	VAL	A	3	16.278	9.497	29.227	1.00	50.25	8

**FIG. 1-19A**

[illegible]

**FIG. 1-19B**

[illegible]

**FIG. 1-19C**

N	SER	A	3	26.013	21.033	22.170	1.00	32.16	7
CA	SER	A	3	26.870	21.550	23.217	1.00	32.60	6
CB	SER	A	3	26.670	20.797	24.533	1.00	33.17	6
O	SER	A	3	26.705	19.395	24.356	1.00	33.68	8
C	SER	A	3	28.342	21.501	22.812	1.00	32.18	6
O	SER	A	3	29.145	22.294	23.305	1.00	32.58	8
N	MET	A	3	28.707	20.593	21.918	1.00	31.37	7
CA	MET	A	3	30.066	20.471	21.421	1.00	30.45	6
CB	MET	A	3	30.467	18.989	21.389	1.00	29.91	6
C	MET	A	3	30.627	18.359	22.763	1.00	30.11	6
SD	MET	A	3	30.676	16.559	22.727	1.00	27.38	1
CE	MET	A	3	28.930	16.174	22.612	1.00	28.29	6
C	MET	A	3	30.209	21.045	20.013	1.00	29.74	6
O	MET	A	3	31.181	21.695	19.643	1.00	30.42	8
N	THR	A	3	29.206	20.776	19.194	1.00	28.53	7
CA	THR	A	3	29.221	21.052	17.764	1.00	26.82	6
CB	THR	A	3	28.529	19.849	17.084	1.00	25.06	6
O	THR	A	3	29.276	19.446	15.930	1.00	30.10	8
C	THR	A	3	27.090	20.114	16.701	1.00	18.67	6
C	THR	A	3	28.614	22.391	17.399	1.00	26.37	6

O	ALA	A	3	21.709	17.524	12.734	1.00	18.70	8
N	GLY	A	3	20.093	18.284	11.392	1.00	18.49	7
CA	GLY	A	3	19.346	17.044	11.340	1.00	18.89	6
C	GLY	A	3	20.085	15.914	10.641	1.00	19.95	6
O	GLY	A	3	19.804	14.742	10.908	1.00	20.23	8
N	ALA	A	3	20.979	16.235	9.714	1.00	20.89	7
CA	ALA	A	3	21.739	15.234	8.980	1.00	22.22	6
CB	ALA	A	3	22.286	15.830	7.690	1.00	20.29	6
C	ALA	A	3	22.879	14.657	9.815	1.00	23.42	6
O	ALA	A	3	22.998	13.436	9.944	1.00	22.82	8
N	VAL	A	3	23.692	15.528	10.413	1.00	23.70	7
CA	VAL	A	3	24.804	15.087	11.243	1.00	24.94	6
CB	VAL	A	3	25.732	16.231	11.691	1.00	24.96	6
C	VAL	A	3	26.375	16.906	10.489	1.00	24.13	6
C	VAL	A	3	25.004	17.259	12.543	1.00	24.96	6
C	VAL	A	3	24.313	14.344	12.482	1.00	25.74	6
O	VAL	A	3	24.898	13.344	12.896	1.00	25.66	8
N	GLU	A	3	23.217	14.813	13.064	1.00	26.47	7
CA	GLU	A	3	22.620	14.235	14.251	1.00	27.57	6
CB	GLU	A	3	21.656	15.256	14.879	1.00	24.46	6

**FIG. 1-20A**

[illegible]

**FIG. 1-20B**





C	ILE	A	3	24.097	5.109	14.695	1.00	32.09	6
O	ILE	A	3	24.031	3.988	15.209	1.00	33.13	8
N	LEU	A	3	25.190	5.860	14.785	1.00	32.34	7
CA	LEU	A	3	26.426	5.390	15.399	1.00	32.59	6
CB	LEU	A	3	27.530	6.448	15.295	1.00	29.08	6
C	LEU	A	3	27.995	6.776	13.872	1.00	28.35	6
C	LEU	A	3	28.988	7.929	13.881	1.00	25.33	6
C	LEU	A	3	28.590	5.552	13.191	1.00	25.41	6
C	LEU	A	3	26.230	4.952	16.840	1.00	33.29	6
O	LEU	A	3	26.799	3.947	17.275	1.00	32.95	8
N	ALA	A	3	25.381	5.648	17.590	1.00	34.07	7
CA	ALA	A	3	25.047	5.296	18.959	1.00	35.50	6
CB	ALA	A	3	24.015	6.269	19.512	1.00	32.60	6
C	ALA	A	3	24.517	3.866	19.051	1.00	36.95	6
O	ALA	A	3	24.828	3.138	19.996	1.00	37.29	8
N	LEU	A	3	23.718	3.445	18.076	1.00	38.32	7
CA	LEU	A	3	23.214	2.088	17.983	1.00	39.35	6
CB	LEU	A	3	22.126	1.997	16.905	1.00	38.88	6
C	LEU	A	3	20.818	2.741	17.188	1.00	39.57	6
C	LEU	A	3	19.876	2.632	15.997	1.00	38.00	6

C	PRO	A	3	25.982	9.912	22.044	1.00	38.43	6
CA	PRO	A	3	27.341	11.232	23.561	1.00	37.39	6
CB	PRO	A	3	27.373	11.879	22.188	1.00	37.81	6
C	PRO	A	3	26.699	10.959	21.245	1.00	38.10	6
C	PRO	A	3	26.686	12.149	24.582	1.00	36.31	6
O	PRO	A	3	25.463	12.195	24.703	1.00	36.61	8
N	PRO	A	3	27.502	12.897	25.314	1.00	34.96	7
C	PRO	A	3	28.985	12.873	25.229	1.00	34.65	6
CA	PRO	A	3	27.030	13.776	26.355	1.00	34.12	6
CB	PRO	A	3	28.269	13.948	27.243	1.00	34.16	6
C	PRO	A	3	29.419	13.827	26.307	1.00	34.54	6
C	PRO	A	3	26.562	15.158	25.945	1.00	33.33	6
O	PRO	A	3	26.823	15.673	24.864	1.00	32.70	8
N	THR	A	3	25.873	15.790	26.892	1.00	33.07	7
CA	THR	A	3	25.505	17.193	26.785	1.00	33.34	6
CB	THR	A	3	24.125	17.525	27.365	1.00	32.36	6
O	THR	A	3	23.125	16.690	26.775	1.00	34.77	8
C	THR	A	3	23.787	18.987	27.116	1.00	30.68	6
C	THR	A	3	26.572	17.928	27.607	1.00	33.64	6
O	THR	A	3	26.393	17.987	28.824	1.00	34.29	8

**FIG. 1-21A**

[illegible]

**FIG. 1-21B**



C	PRO	A	3	20.703	19.878	36.120	1.00	57.10	6
C	PRO	A	3	18.996	23.049	35.491	1.00	60.26	6
O	PRO	A	3	19.009	23.592	36.597	1.00	60.43	8
N	ASP	A	3	18.120	23.370	34.544	1.00	62.72	7
CA	ASP	A	3	17.091	24.389	34.766	1.00	65.42	6
CB	ASP	A	3	16.358	24.680	33.461	1.00	65.96	6
C	ASP	A	3	15.930	26.125	33.310	1.00	66.13	6
O	ASP	A	3	16.724	27.026	33.650	1.00	66.02	8
O	ASP	A	3	14.791	26.358	32.850	1.00	66.29	8
C	ASP	A	3	16.146	23.894	35.856	1.00	67.55	6
O	ASP	A	3	16.062	22.683	36.086	1.00	67.61	8
N	GLU	A	3	15.435	24.785	36.534	1.00	69.63	7
CA	GLU	A	3	14.574	24.425	37.650	1.00	71.91	6
CB	GLU	A	3	13.891	25.670	38.236	1.00	75.55	6
C	GLU	A	3	12.875	26.305	37.311	1.00	80.01	6
C	GLU	A	3	11.769	27.059	38.015	1.00	82.31	6
O	GLU	A	3	10.586	26.784	37.716	1.00	83.41	8
O	GLU	A	3	12.072	27.930	38.856	1.00	83.82	8
O	PHE	A	3	22.597	14.874	28.844	1.00	40.83	8
N	VAL	A	3	22.307	12.972	29.970	1.00	40.72	7
CA	VAL	A	3	23.650	12.448	29.776	1.00	40.16	6
CB	VAL	A	3	23.891	11.815	28.403	1.00	38.09	6
C	VAL	A	3	25.173	10.990	28.427	1.00	36.99	6
C	VAL	A	3	22.727	10.932	27.974	1.00	38.10	6
C	VAL	A	3	24.659	13.563	30.056	1.00	40.38	6
O	VAL	A	3	25.385	14.035	29.186	1.00	40.38	8
N	PRO	A	3	24.700	14.009	31.313	1.00	40.78	7
C	PRO	A	3	23.800	13.524	32.404	1.00	40.85	6
CA	PRO	A	3	25.309	15.254	31.696	1.00	40.90	6
CB	PRO	A	3	25.114	15.342	33.216	1.00	40.96	6
C	PRO	A	3	24.428	14.100	33.638	1.00	40.79	6
C	PRO	A	3	26.734	15.593	31.358	1.00	41.19	6
O	PRO	A	3	26.904	16.768	30.971	1.00	42.24	8
N	HIS	A	3	27.780	14.807	31.590	1.00	40.96	7
CA	HIS	A	3	29.125	15.321	31.308	1.00	40.86	6
CB	HIS	A	3	29.855	15.671	32.615	1.00	40.66	6

**FIG. 1-22A**





C	VAL	A	3	24.491	-0.100	26.668	1.00	38.94	6
O	VAL	A	3	25.540	-0.387	26.081	1.00	38.81	8
N	SER	A	3	23.501	-0.967	26.865	1.00	39.38	7
CA	SER	A	3	23.663	-2.356	26.464	1.00	40.73	6
CB	SER	A	3	23.649	-3.252	27.720	1.00	40.55	6
O	SER	A	3	23.861	-4.601	27.327	1.00	42.48	8
C	SER	A	3	22.681	-2.919	25.456	1.00	41.20	6
O	SER	A	3	23.144	-3.476	24.447	1.00	41.74	8
N	GLY	A	3	21.377	-2.851	25.686	1.00	41.13	7
CA	GLY	A	3	20.429	-3.435	24.741	1.00	42.12	6
C	GLY	A	3	19.550	-2.401	24.054	1.00	42.75	6
O	GLY	A	3	18.326	-2.538	24.022	1.00	42.94	8
N	MET	A	3	20.167	-1.367	23.500	1.00	43.16	7
CA	MET	A	3	19.440	-0.299	22.822	1.00	43.71	6
CB	MET	A	3	20.230	1.004	22.944	1.00	43.69	6
C	MET	A	3	19.642	2.207	22.232	1.00	43.01	6
SD	MET	A	3	20.366	3.767	22.774	1.00	43.68	1
CE	MET	A	3	21.976	3.688	21.993	1.00	42.01	6
C	MET	A	3	19.192	-0.651	21.361	1.00	44.30	6
O	MET	A	3	20.141	-0.930	20.627	1.00	44.01	8

CB	ASN	A	3	14.226	15.790	18.260	1.00	36.16	6
C	ASN	A	3	13.048	14.951	18.697	1.00	39.16	6
O	ASN	A	3	12.375	14.313	17.887	1.00	41.53	8
N	ASN	A	3	12.774	14.966	19.997	1.00	39.24	7
C	ASN	A	3	15.191	16.827	16.233	1.00	32.97	6
O	ASN	A	3	16.246	17.325	16.617	1.00	32.75	8
N	SER	A	3	14.373	17.483	15.413	1.00	32.66	7
CA	SER	A	3	14.676	18.793	14.851	1.00	31.74	6
CB	SER	A	3	15.200	18.682	13.422	1.00	31.39	6
O	SER	A	3	16.598	18.874	13.359	1.00	31.26	8
C	SER	A	3	13.416	19.656	14.860	1.00	31.57	6
O	SER	A	3	12.435	19.319	14.194	1.00	31.75	8
N	PHE	A	3	13.415	20.722	15.649	1.00	30.83	7
CA	PHE	A	3	12.270	21.619	15.761	1.00	31.51	6
CB	PHE	A	3	11.712	21.643	17.185	1.00	31.46	6
C	PHE	A	3	11.529	20.317	17.862	1.00	32.87	6
C	PHE	A	3	12.125	20.065	19.087	1.00	33.75	6
C	PHE	A	3	10.774	19.310	17.280	1.00	33.53	6
CE	PHE	A	3	11.976	18.843	19.714	1.00	33.89	6
CE	PHE	A	3	10.633	18.082	17.894	1.00	35.78	6

**FIG. 1-23A**

[illegible]

**FIG. 1-23B**





O	GLY	A	4	11.944	16.126	14.327	1.00	27.32	8
N	SER	A	4	10.927	14.377	13.367	1.00	27.36	7
CA	SER	A	4	11.586	13.366	14.170	1.00	28.27	6
CB	SER	A	4	10.743	12.925	15.365	1.00	28.64	6
O	SER	A	4	10.364	13.975	16.224	1.00	26.79	8
C	SER	A	4	11.856	12.135	13.302	1.00	28.72	6
O	SER	A	4	11.003	11.766	12.495	1.00	29.31	8
N	LEU	A	4	13.016	11.523	13.484	1.00	28.57	7
CA	LEU	A	4	13.348	10.304	12.751	1.00	28.67	6
CB	LEU	A	4	14.534	10.504	11.819	1.00	26.79	6
C	LEU	A	4	14.245	11.209	10.488	1.00	28.09	6
C	LEU	A	4	15.526	11.739	9.863	1.00	26.35	6
C	LEU	A	4	13.529	10.278	9.521	1.00	26.42	6
C	LEU	A	4	13.600	9.198	13.777	1.00	29.89	6
O	LEU	A	4	14.008	9.492	14.906	1.00	30.25	8
N	ILE	A	4	13.195	7.972	13.474	1.00	30.42	7
CA	ILE	A	4	13.409	6.837	14.359	1.00	31.78	6
CB	ILE	A	4	12.123	6.165	14.866	1.00	30.94	6
C	ILE	A	4	12.444	4.865	15.599	1.00	32.61	6
C	ILE	A	4	11.340	7.091	15.798	1.00	30.59	6
C	ILE	A	4	10.007	6.541	16.250	1.00	32.84	6
C	ILE	A	4	14.260	5.794	13.630	1.00	33.11	6

O1	WAT	W	5	24.648	28.103	4.390	1.00	24.17	8
O1	WAT	W	5	24.853	18.181	17.061	1.00	21.49	8
O1	WAT	W	5	15.266	27.397	5.435	1.00	23.74	8
O1	WAT	W	5	29.879	26.729	23.056	1.00	27.80	8
O1	WAT	W	5	8.228	26.466	7.960	1.00	28.01	8
O1	WAT	W	5	25.350	-0.832	-1.565	1.00	33.85	8
O1	WAT	W	5	23.401	42.296	15.101	1.00	39.31	8
O1	WAT	W	5	22.521	37.586	20.198	1.00	39.72	8
O1	WAT	W	5	35.693	38.967	-9.343	1.00	45.45	8
O1	WAT	W	5	8.464	1.674	8.701	1.00	48.55	8
O1	WAT	W	5	14.310	29.899	19.439	1.00	43.00	8
O1	WAT	W	5	10.440	4.010	6.351	1.00	41.78	8
O1	WAT	W	5	9.624	13.271	34.855	1.00	46.76	8
O1	WAT	W	5	31.169	43.463	9.374	1.00	48.95	8
O1	WAT	W	5	37.224	13.856	2.117	1.00	48.60	8
O1	WAT	W	5	0.645	16.105	12.588	1.00	51.59	8
O1	WAT	W	5	1.627	11.628	29.727	1.00	42.16	8
O1	WAT	W	5	13.937	1.427	26.436	1.00	51.44	8
O1	WAT	W	5	30.994	42.927	5.494	1.00	51.60	8
O1	WAT	W	5	31.903	36.386	2.731	1.00	52.75	8
O1	WAT	W	5	8.997	5.935	-10.232	1.00	49.23	8
O1	WAT	W	5	41.291	24.980	-1.863	1.00	52.73	8

**FIG. 1-24A**





N	ARG	B	4	-11.838	10.004	-7.911	0.00	0.00	7	CA	SER	B	1	0.573	37.004	-11.205	0.00	0.00	6
C	ARG	B	4	-6.886	11.333	-3.435	0.00	0.00	6	CB	SER	B	1	-0.015	35.962	-12.155	0.00	0.00	6
O	ARG	B	4	-7.460	11.712	-2.416	0.00	0.00	8	O	SER	B	1	-0.875	36.553	-13.112	0.00	0.00	8
N	VAL	B	5	-6.150	12.141	-4.194	0.00	0.00	7	C	SER	B	1	0.707	38.350	-11.895	0.00	0.00	6
CA	VAL	B	5	-5.980	13.555	-3.891	0.00	0.00	6	O	SER	B	1	-0.036	39.287	-11.612	0.00	0.00	8
CB	VAL	B	5	-4.499	13.967	-3.796	0.00	0.00	6	N	PRO	B	1	1.592	38.431	-12.880	0.00	0.00	7
C	VAL	B	5	-4.375	15.410	-3.320	0.00	0.00	6	C	PRO	B	1	2.528	37.351	-13.288	0.00	0.00	6
C	VAL	B	5	-3.712	13.046	-2.877	0.00	0.00	6	CA	PRO	B	1	1.796	39.632	-13.665	0.00	0.00	6
C	VAL	B	5	-6.649	14.423	-4.953	0.00	0.00	6	CB	PRO	B	1	3.008	39.317	-14.535	0.00	0.00	6
O	VAL	B	5	-6.439	14.236	-6.151	0.00	0.00	8	C	PRO	B	1	3.661	38.139	-13.902	0.00	0.00	6
N	VAL	B	6	-7.458	15.377	-4.506	0.00	0.00	7	C	PRO	B	1	0.602	40.043	-14.509	0.00	0.00	6
CA	VAL	B	6	-8.162	16.289	-5.394	0.00	0.00	6	O	PRO	B	1	0.561	41.209	-14.924	0.00	0.00	8
CB	VAL	B	6	-9.689	16.096	-5.351	0.00	0.00	6	N	VAL	B	1	-0.355	39.168	-14.817	0.00	0.00	7
C	VAL	B	6	-10.108	14.791	-6.013	0.00	0.00	6	CA	VAL	B	1	-1.521	39.561	-15.592	0.00	0.00	6
C	VAL	B	6	-10.207	16.146	-3.921	0.00	0.00	6	CB	VAL	B	1	-1.781	38.692	-16.836	0.00	0.00	6
C	VAL	B	6	-7.835	17.739	-5.044	0.00	0.00	6	C	VAL	B	1	-0.708	38.926	-17.890	0.00	0.00	6
O	VAL	B	6	-7.351	18.031	-3.954	0.00	0.00	8	C	VAL	B	1	-1.882	37.219	-16.477	0.00	0.00	6
N	VAL	B	7	-8.082	18.647	-5.981	0.00	0.00	7	C	VAL	B	1	-2.799	39.600	-14.761	0.00	0.00	6
CA	VAL	B	7	-7.829	20.072	-5.781	0.00	0.00	6	O	VAL	B	1	-3.883	39.725	-15.340	0.00	0.00	8
CB	VAL	B	7	-7.171	20.707	-7.016	0.00	0.00	6	N	GLY	B	1	-2.703	39.502	-13.440	0.00	0.00	7

**FIG. 1-25A**





C	THR	B	2	-3.400	34.381	-14.101	0.00	0.00	6
C	THR	B	2	-5.685	35.070	-15.601	0.00	0.00	6
O	THR	B	2	-5.100	35.126	-16.681	0.00	0.00	8
N	TRP	B	2	-6.625	34.166	-15.337	0.00	0.00	7
CA	TRP	B	2	-7.069	33.187	-16.324	0.00	0.00	6
CB	TRP	B	2	-8.124	32.257	-15.721	0.00	0.00	6
C	TRP	B	2	-8.554	31.131	-16.610	0.00	0.00	6
C	TRP	B	2	-7.715	30.225	-17.335	0.00	0.00	6
CE	TRP	B	2	-8.556	29.338	-18.035	0.00	0.00	6
CE	TRP	B	2	-6.330	30.079	-17.462	0.00	0.00	6
C	TRP	B	2	-9.839	30.763	-16.892	0.00	0.00	6
N	TRP	B	2	-9.849	29.686	-17.746	0.00	0.00	7
CZ	TRP	B	2	-8.062	28.322	-18.849	0.00	0.00	6
CZ	TRP	B	2	-5.840	29.069	-18.269	0.00	0.00	6
C	TRP	B	2	-6.704	28.201	-18.952	0.00	0.00	6
C	TRP	B	2	-7.583	33.858	-17.592	0.00	0.00	6
O	TRP	B	2	-7.160	33.508	-18.694	0.00	0.00	8
N	LYS	B	2	-8.470	34.834	-17.456	0.00	0.00	7
CA	LYS	B	2	-9.042	35.564	-18.576	0.00	0.00	6
CB	LYS	B	2	-10.109	36.555	-18.097	0.00	0.00	6

O	GLN	B	3	-0.765	38.310	-21.429	0.00	0.00	8
N	SER	B	3	-0.062	40.251	-22.307	0.00	0.00	7
CA	SER	B	3	1.278	40.169	-21.739	0.00	0.00	6
CB	SER	B	3	2.294	40.807	-22.679	0.00	0.00	6
O	SER	B	3	3.597	40.831	-22.140	0.00	0.00	8
C	SER	B	3	1.274	40.874	-20.386	0.00	0.00	6
O	SER	B	3	0.498	41.811	-20.191	0.00	0.00	8
N	GLY	B	3	2.110	40.424	-19.459	0.00	0.00	7
CA	GLY	B	3	2.170	41.044	-18.135	0.00	0.00	6
C	GLY	B	3	3.536	41.687	-17.921	0.00	0.00	6
O	GLY	B	3	3.897	42.130	-16.835	0.00	0.00	8
N	ILE	B	3	4.303	41.749	-19.000	0.00	0.00	7
CA	ILE	B	3	5.671	42.238	-18.997	0.00	0.00	6
CB	ILE	B	3	6.473	41.482	-20.089	0.00	0.00	6
C	ILE	B	3	7.954	41.783	-19.950	0.00	0.00	6
C	ILE	B	3	6.125	40.003	-19.990	0.00	0.00	6
C	ILE	B	3	7.148	38.944	-20.253	0.00	0.00	6
C	ILE	B	3	5.778	43.741	-19.184	0.00	0.00	6
O	ILE	B	3	5.345	44.318	-20.180	0.00	0.00	8
N	SER	B	3	6.393	44.396	-18.204	0.00	0.00	7

**FIG. 1-26A**



[illegible]

**FIG. 1-26B**



C	PHE	B	4	17.120	48.028	-10.416	0.00	0.00	6
CE	PHE	B	4	15.281	46.015	-10.000	0.00	0.00	6
CE	PHE	B	4	17.184	46.867	-11.163	0.00	0.00	6
CZ	PHE	B	4	16.264	45.859	-10.957	0.00	0.00	6
C	PHE	B	4	15.893	51.121	-10.527	0.00	0.00	6
O	PHE	B	4	15.265	50.943	-11.571	0.00	0.00	8
N	ASP	B	4	17.003	51.846	-10.472	0.00	0.00	7
CA	ASP	B	4	17.611	52.372	-11.690	0.00	0.00	6
CB	ASP	B	4	18.687	53.406	-11.349	0.00	0.00	6
C	ASP	B	4	18.923	54.376	-12.491	0.00	0.00	6
O	ASP	B	4	17.932	54.804	-13.121	0.00	0.00	8
O	ASP	B	4	20.095	54.711	-12.759	0.00	0.00	8
C	ASP	B	4	18.201	51.255	-12.541	0.00	0.00	6
O	ASP	B	4	19.158	50.593	-12.140	0.00	0.00	8
N	THR	B	4	17.644	51.053	-13.732	0.00	0.00	7
CA	THR	B	4	18.114	50.015	-14.639	0.00	0.00	6
CB	THR	B	4	16.921	49.251	-15.254	0.00	0.00	6
O	THR	B	4	16.088	50.174	-15.962	0.00	0.00	8
C	THR	B	4	16.100	48.566	-14.175	0.00	0.00	6
C	THR	B	4	19.000	50.539	-15.760	0.00	0.00	6

O	LYS	B	4	13.002	47.106	-17.414	0.00	0.00	8
N	PHE	B	4	13.301	45.009	-18.189	0.00	0.00	7
CA	PHE	B	4	11.887	44.672	-18.067	0.00	0.00	6
CB	PHE	B	4	11.267	44.557	-19.465	0.00	0.00	6
C	PHE	B	4	11.965	43.566	-20.352	0.00	0.00	6
C	PHE	B	4	11.550	42.247	-20.404	0.00	0.00	6
C	PHE	B	4	13.041	43.957	-21.135	0.00	0.00	6
CE	PHE	B	4	12.192	41.332	-21.220	0.00	0.00	6
CE	PHE	B	4	13.689	43.046	-21.946	0.00	0.00	6
CZ	PHE	B	4	13.260	41.735	-21.996	0.00	0.00	6
C	PHE	B	4	11.666	43.382	-17.292	0.00	0.00	6
O	PHE	B	4	12.576	42.577	-17.108	0.00	0.00	8
N	ALA	B	5	10.424	43.181	-16.864	0.00	0.00	7
CA	ALA	B	5	10.032	41.986	-16.135	0.00	0.00	6
CB	ALA	B	5	10.666	41.977	-14.749	0.00	0.00	6
C	ALA	B	5	8.513	41.888	-16.010	0.00	0.00	6
O	ALA	B	5	7.772	42.820	-16.314	0.00	0.00	8
N	GLY	B	5	8.060	40.724	-15.560	0.00	0.00	7
CA	GLY	B	5	6.631	40.512	-15.301	0.00	0.00	6
C	GLY	B	5	6.446	40.886	-13.820	0.00	0.00	6

**FIG. 1-27A**





N	ASN	B	5	-2.151	45.071	-3.051	0.00	0.00	7
CA	ASN	B	5	-2.663	45.532	-1.769	0.00	0.00	6
CB	ASN	B	5	-3.948	46.342	-1.930	0.00	0.00	6
C	ASN	B	5	-4.421	46.975	-0.637	0.00	0.00	6
O	ASN	B	5	-5.590	46.855	-0.266	0.00	0.00	8
N	ASN	B	5	-3.525	47.660	0.065	0.00	0.00	7
C	ASN	B	5	-2.914	44.343	-0.842	0.00	0.00	6
O	ASN	B	5	-3.604	43.391	-1.203	0.00	0.00	8
N	CYS	B	5	-2.309	44.399	0.338	0.00	0.00	7
CA	CYS	B	5	-2.467	43.334	1.322	0.00	0.00	6
CB	CYS	B	5	-1.236	42.431	1.347	0.00	0.00	6
SG	CYS	B	5	0.252	43.226	1.997	0.00	0.00	1
C	CYS	B	5	-2.728	43.929	2.699	0.00	0.00	6
O	CYS	B	5	-2.729	43.232	3.709	0.00	0.00	8
N	GLU	B	5	-3.065	45.214	2.722	0.00	0.00	7
CA	GLU	B	5	-3.394	45.936	3.943	0.00	0.00	6
CB	GLU	B	5	-3.775	47.378	3.604	0.00	0.00	6
C	GLU	B	5	-3.621	48.366	4.743	0.00	0.00	6
C	GLU	B	5	-2.414	49.271	4.612	0.00	0.00	6
O	GLU	B	5	-2.406	50.339	5.266	0.00	0.00	8

N	LYS	B	6	2.286	47.070	10.259	0.00	0.00	7
CA	LYS	B	6	3.206	46.697	11.323	0.00	0.00	6
CB	LYS	B	6	2.497	46.565	12.667	0.00	0.00	6
C	LYS	B	6	1.922	47.844	13.247	0.00	0.00	6
C	LYS	B	6	0.962	47.542	14.390	0.00	0.00	6
CE	LYS	B	6	-0.211	48.508	14.405	0.00	0.00	6
NZ	LYS	B	6	-1.501	47.832	14.094	0.00	0.00	7
C	LYS	B	6	3.836	45.348	10.959	0.00	0.00	6
O	LYS	B	6	5.053	45.206	10.893	0.00	0.00	8
N	GLU	B	6	2.985	44.370	10.663	0.00	0.00	7
CA	GLU	B	6	3.403	43.026	10.303	0.00	0.00	6
CB	GLU	B	6	2.191	42.084	10.348	0.00	0.00	6
C	GLU	B	6	1.842	41.634	11.759	0.00	0.00	6
C	GLU	B	6	2.805	40.594	12.296	0.00	0.00	6
O	GLU	B	6	3.270	40.746	13.444	0.00	0.00	8
O	GLU	B	6	3.100	39.622	11.571	0.00	0.00	8
C	GLU	B	6	4.103	42.913	8.961	0.00	0.00	6
O	GLU	B	6	4.935	42.026	8.749	0.00	0.00	8
N	GLN	B	6	3.833	43.819	8.034	0.00	0.00	7
CA	GLN	B	6	4.432	43.873	6.715	0.00	0.00	6

**FIG. 1-28A**







CA	ALA	B	7	7.671	40.673	-0.831	0.00	0.00	6
CB	ALA	B	7	8.021	41.490	-2.079	0.00	0.00	6
C	ALA	B	7	7.259	39.269	-1.251	0.00	0.00	6
O	ALA	B	7	6.061	39.058	-1.483	0.00	0.00	8
N	PHE	B	7	8.176	38.313	-1.373	0.00	0.00	7
CA	PHE	B	7	7.811	36.950	-1.753	0.00	0.00	6
CB	PHE	B	7	9.022	36.071	-2.038	0.00	0.00	6
C	PHE	B	7	9.565	35.217	-0.936	0.00	0.00	6
C	PHE	B	7	9.197	33.886	-0.811	0.00	0.00	6
C	PHE	B	7	10.450	35.738	-0.006	0.00	0.00	6
CE	PHE	B	7	9.696	33.100	0.210	0.00	0.00	6
CE	PHE	B	7	10.948	34.963	1.024	0.00	0.00	6
CZ	PHE	B	7	10.580	33.638	1.126	0.00	0.00	6
C	PHE	B	7	6.893	36.327	-0.705	0.00	0.00	6
O	PHE	B	7	5.933	35.641	-1.064	0.00	0.00	8
N	ILE	B	7	7.163	36.563	0.574	0.00	0.00	7
CA	ILE	B	7	6.304	36.067	1.645	0.00	0.00	6
CB	ILE	B	7	6.972	36.219	3.022	0.00	0.00	6
C	ILE	B	7	6.000	35.961	4.164	0.00	0.00	6
C	ILE	B	7	8.162	35.254	3.121	0.00	0.00	6

CA	ALA	B	8	-2.383	33.822	-2.558	0.00	0.00	6
CB	ALA	B	8	-1.272	33.385	-3.500	0.00	0.00	6
C	ALA	B	8	-2.843	32.640	-1.711	0.00	0.00	6
O	ALA	B	8	-3.746	31.904	-2.112	0.00	0.00	8
N	GLY	B	8	-2.218	32.434	-0.555	0.00	0.00	7
CA	GLY	B	8	-2.604	31.380	0.370	0.00	0.00	6
C	GLY	B	8	-3.981	31.650	0.965	0.00	0.00	6
O	GLY	B	8	-4.833	30.763	1.014	0.00	0.00	8
N	VAL	B	8	-4.230	32.898	1.357	0.00	0.00	7
CA	VAL	B	8	-5.528	33.288	1.897	0.00	0.00	6
CB	VAL	B	8	-5.532	34.736	2.405	0.00	0.00	6
C	VAL	B	8	-6.925	35.177	2.836	0.00	0.00	6
C	VAL	B	8	-4.556	34.880	3.570	0.00	0.00	6
C	VAL	B	8	-6.620	33.064	0.859	0.00	0.00	6
O	VAL	B	8	-7.659	32.482	1.179	0.00	0.00	8
N	GLN	B	8	-6.364	33.415	-0.397	0.00	0.00	7
CA	GLN	B	8	-7.290	33.149	-1.485	0.00	0.00	6
CB	GLN	B	8	-6.721	33.632	-2.822	0.00	0.00	6
C	GLN	B	8	-6.689	35.138	-3.007	0.00	0.00	6
C	GLN	B	8	-6.219	35.543	-4.389	0.00	0.00	6

**FIG. 1-29A**

C	ILE	B	7	9.131	35.593	4.232	0.00	0.00	6
C	ILE	B	7	4.949	36.764	1.611	0.00	0.00	6
O	ILE	B	7	3.917	36.114	1.777	0.00	0.00	8
N	GLN	B	7	4.940	38.071	1.364	0.00	0.00	7
CA	GLN	B	7	3.695	38.826	1.257	0.00	0.00	6
CB	GLN	B	7	3.976	40.311	1.047	0.00	0.00	6
C	GLN	B	7	4.678	40.988	2.211	0.00	0.00	6
C	GLN	B	7	4.908	42.469	1.984	0.00	0.00	6
O	GLN	B	7	4.269	43.091	1.131	0.00	0.00	8
N	GLN	B	7	5.823	43.047	2.755	0.00	0.00	7
C	GLN	B	7	2.836	38.275	0.122	0.00	0.00	6
O	GLN	B	7	1.645	38.009	0.314	0.00	0.00	8
N	TYR	B	7	3.435	38.020	-1.038	0.00	0.00	7
CA	TYR	B	7	2.730	37.400	-2.151	0.00	0.00	6
CB	TYR	B	7	3.639	37.244	-3.365	0.00	0.00	6
C	TYR	B	7	4.073	38.496	-4.083	0.00	0.00	6
C	TYR	B	7	4.947	38.395	-5.163	0.00	0.00	6
CE	TYR	B	7	5.370	39.516	-5.853	0.00	0.00	6
C	TYR	B	7	3.645	39.764	-3.717	0.00	0.00	6
CE	TYR	B	7	4.069	40.894	-4.390	0.00	0.00	6
CZ	TYR	B	7	4.932	40.761	-5.457	0.00	0.00	6
O	GLN	B	8	-6.176	34.726	-5.309	0.00	0.00	8
N	GLN	B	8	-5.860	36.811	-4.554	0.00	0.00	7
C	GLN	B	8	-7.631	31.667	-1.602	0.00	0.00	6
O	GLN	B	8	-8.802	31.315	-1.758	0.00	0.00	8
N	ALA	B	8	-6.629	30.793	-1.539	0.00	0.00	7
CA	ALA	B	8	-6.857	29.358	-1.660	0.00	0.00	6
CB	ALA	B	8	-5.541	28.617	-1.828	0.00	0.00	6
C	ALA	B	8	-7.647	28.802	-0.484	0.00	0.00	6
O	ALA	B	8	-8.519	27.949	-0.673	0.00	0.00	8
N	MET	B	8	-7.360	29.274	0.724	0.00	0.00	7
CA	MET	B	8	-8.113	28.856	1.902	0.00	0.00	6
CB	MET	B	8	-7.490	29.432	3.172	0.00	0.00	6
C	MET	B	8	-6.228	28.709	3.621	0.00	0.00	6
SD	MET	B	8	-6.445	26.925	3.753	0.00	0.00	1
CE	MET	B	8	-6.387	26.701	5.528	0.00	0.00	6
C	MET	B	8	-9.574	29.266	1.757	0.00	0.00	6
O	MET	B	8	-10.478	28.445	1.919	0.00	0.00	8
N	GLN	B	8	-9.809	30.522	1.397	0.00	0.00	7
CA	GLN	B	8	-11.155	31.043	1.192	0.00	0.00	6
CB	GLN	B	8	-11.101	32.552	0.925	0.00	0.00	6
C	GLN	B	8	-10.844	33.369	2.182	0.00	0.00	6

**FIG. 1-29B**



N	LEU	B	9	-12.800	25.551	3.826	0.00	0.00	7
CA	LEU	B	9	-12.265	24.680	4.861	0.00	0.00	6
CB	LEU	B	9	-10.779	24.409	4.677	0.00	0.00	6
C	LEU	B	9	-10.302	22.986	4.394	0.00	0.00	6
C	LEU	B	9	-10.926	21.966	5.334	0.00	0.00	6
C	LEU	B	9	-10.574	22.608	2.943	0.00	0.00	6
C	LEU	B	9	-12.507	25.349	6.216	0.00	0.00	6
O	LEU	B	9	-12.209	26.531	6.384	0.00	0.00	8
N	GLU	B	9	-13.164	24.627	7.112	0.00	0.00	7
CA	GLU	B	9	-13.346	25.130	8.474	0.00	0.00	6
CB	GLU	B	9	-14.753	24.868	8.989	0.00	0.00	6
C	GLU	B	9	-15.849	25.580	8.213	0.00	0.00	6
C	GLU	B	9	-16.839	26.303	9.104	0.00	0.00	6
O	GLU	B	9	-17.285	25.715	10.113	0.00	0.00	8
O	GLU	B	9	-17.179	27.465	8.797	0.00	0.00	8
C	GLU	B	9	-12.279	24.461	9.339	0.00	0.00	6
O	GLU	B	9	-12.201	23.231	9.355	0.00	0.00	8
N	ILE	B	9	-11.401	25.263	9.933	0.00	0.00	7
CA	ILE	B	9	-10.330	24.696	10.753	0.00	0.00	6
CB	ILE	B	9	-9.003	25.449	10.595	0.00	0.00	6

CA	THR	B	9	-3.494	18.120	13.183	0.00	0.00	6
CB	THR	B	9	-3.849	17.091	14.293	0.00	0.00	6
O	THR	B	9	-3.158	17.483	15.494	0.00	0.00	8
C	THR	B	9	-3.510	15.649	13.985	0.00	0.00	6
C	THR	B	9	-3.392	17.455	11.826	0.00	0.00	6
O	THR	B	9	-2.336	16.879	11.520	0.00	0.00	8
N	ARG	B	9	-4.417	17.469	10.983	0.00	0.00	7
CA	ARG	B	9	-4.390	16.835	9.680	0.00	0.00	6
CB	ARG	B	9	-5.674	16.018	9.462	0.00	0.00	6
C	ARG	B	9	-5.976	14.996	10.544	0.00	0.00	6
C	ARG	B	9	-4.989	13.839	10.499	0.00	0.00	6
N	ARG	B	9	-5.164	13.029	9.300	0.00	0.00	7
CZ	ARG	B	9	-4.248	12.221	8.785	0.00	0.00	6
N	ARG	B	9	-3.058	12.093	9.357	0.00	0.00	7
N	ARG	B	9	-4.525	11.530	7.686	0.00	0.00	7
C	ARG	B	9	-4.224	17.795	8.512	0.00	0.00	6
O	ARG	B	9	-4.283	17.365	7.356	0.00	0.00	8
N	ILE	B	1	-4.106	19.091	8.777	0.00	0.00	7
CA	ILE	B	1	-3.917	20.072	7.716	0.00	0.00	6
CB	ILE	B	1	-4.981	21.183	7.700	0.00	0.00	6

**FIG. 1-30A**

[illegible]

**FIG. 1-30B**



C	ILE	B	1	16.794	34.404	-4.750	0.00	0.00	0.00	6
C	ILE	B	1	16.591	32.700	-6.544	0.00	0.00	0.00	6
C	ILE	B	1	16.491	33.542	-7.796	0.00	0.00	0.00	6
C	ILE	B	1	15.199	32.836	-2.938	0.00	0.00	0.00	6
O	ILE	B	1	16.082	33.200	-2.153	0.00	0.00	0.00	8
N	GLY	B	1	13.913	32.958	-2.623	0.00	0.00	0.00	7
CA	GLY	B	1	13.500	33.524	-1.345	0.00	0.00	0.00	6
C	GLY	B	1	13.749	35.023	-1.274	0.00	0.00	0.00	6
O	GLY	B	1	13.728	35.733	-2.279	0.00	0.00	0.00	8
N	GLY	B	1	13.868	35.559	-0.062	0.00	0.00	0.00	7
CA	GLY	B	1	13.870	36.971	0.218	0.00	0.00	0.00	6
C	GLY	B	1	15.050	37.802	-0.223	0.00	0.00	0.00	6
O	GLY	B	1	15.661	38.511	0.585	0.00	0.00	0.00	8
N	LEU	B	1	15.285	37.900	-1.526	0.00	0.00	0.00	7
CA	LEU	B	1	16.398	38.625	-2.104	0.00	0.00	0.00	6
CB	LEU	B	1	16.437	38.408	-3.622	0.00	0.00	0.00	6
C	LEU	B	1	17.663	37.729	-4.225	0.00	0.00	0.00	6
C	LEU	B	1	17.647	37.859	-5.744	0.00	0.00	0.00	6
C	LEU	B	1	18.962	38.287	-3.670	0.00	0.00	0.00	6
C	LEU	B	1	16.332	40.119	-1.822	0.00	0.00	0.00	6

N	ASN	B	1	17.280	42.501	5.940	0.00	0.00	0.00	7
C	ASN	B	1	21.570	44.367	4.958	0.00	0.00	0.00	6
O	ASN	B	1	22.333	44.848	5.801	0.00	0.00	0.00	8
N	HIS	B	1	22.005	43.840	3.811	0.00	0.00	0.00	7
CA	HIS	B	1	23.431	43.856	3.503	0.00	0.00	0.00	6
CB	HIS	B	1	23.819	43.004	2.295	0.00	0.00	0.00	6
C	HIS	B	1	25.315	42.861	2.216	0.00	0.00	0.00	6
C	HIS	B	1	26.222	43.348	1.343	0.00	0.00	0.00	6
N	HIS	B	1	26.030	42.144	3.151	0.00	0.00	0.00	7
CE	HIS	B	1	27.316	42.190	2.852	0.00	0.00	0.00	6
N	HIS	B	1	27.457	42.915	1.755	0.00	0.00	0.00	7
C	HIS	B	1	23.889	45.303	3.321	0.00	0.00	0.00	6
O	HIS	B	1	24.898	45.713	3.898	0.00	0.00	0.00	8
N	THR	B	1	23.091	46.103	2.620	0.00	0.00	0.00	7
CA	THR	B	1	23.383	47.523	2.448	0.00	0.00	0.00	6
CB	THR	B	1	22.322	48.196	1.562	0.00	0.00	0.00	6
O	THR	B	1	22.311	47.533	0.288	0.00	0.00	0.00	8
C	THR	B	1	22.621	49.671	1.345	0.00	0.00	0.00	6
C	THR	B	1	23.500	48.228	3.792	0.00	0.00	0.00	6
O	THR	B	1	24.478	48.942	4.033	0.00	0.00	0.00	8

**FIG. 1-31A**

	O	LEU	B	1	17.336	40.749	-1.493	0.00	0.00	8		N	SER	B	1	22.553	47.994	4.695	0.00	0.00	7
	N	GLY	B	1	15.138	40.687	-1.966	0.00	0.00	7		CA	SER	B	1	22.625	48.540	6.047	0.00	0.00	6
	CA	GLY	B	1	14.920	42.106	-1.717	0.00	0.00	6		CB	SER	B	1	21.426	48.068	6.870	0.00	0.00	6
	C	GLY	B	1	15.413	42.510	-0.333	0.00	0.00	6		O	SER	B	1	20.215	48.456	6.236	0.00	0.00	8
	O	GLY	B	1	16.245	43.408	-0.215	0.00	0.00	8		C	SER	B	1	23.939	48.154	6.711	0.00	0.00	6
	N	LEU	B	1	15.004	41.772	0.696	0.00	0.00	7		O	SER	B	1	24.722	49.019	7.100	0.00	0.00	8
	CA	LEU	B	1	15.384	42.075	2.069	0.00	0.00	6		N	LEU	B	1	24.244	46.863	6.777	0.00	0.00	7
	CB	LEU	B	1	14.380	41.456	3.045	0.00	0.00	6		CA	LEU	B	1	25.484	46.363	7.350	0.00	0.00	6
	C	LEU	B	1	13.469	42.434	3.794	0.00	0.00	6		CB	LEU	B	1	25.569	44.846	7.172	0.00	0.00	6
	C	LEU	B	1	12.982	43.576	2.917	0.00	0.00	6		C	LEU	B	1	26.914	44.158	7.405	0.00	0.00	6
	C	LEU	B	1	12.272	41.709	4.396	0.00	0.00	6		C	LEU	B	1	27.242	44.061	8.887	0.00	0.00	6
	C	LEU	B	1	16.822	41.718	2.403	0.00	0.00	6		C	LEU	B	1	26.922	42.773	6.770	0.00	0.00	6
	O	LEU	B	1	17.408	42.358	3.288	0.00	0.00	8		C	LEU	B	1	26.720	47.037	6.775	0.00	0.00	6
	N	I LE	B	1	17.433	40.762	1.707	0.00	0.00	7		O	LEU	B	1	27.612	47.426	7.535	0.00	0.00	8
	CA	I LE	B	1	18.834	40.428	1.959	0.00	0.00	6		N	MET	B	1	26.808	47.199	5.461	0.00	0.00	7
	CB	I LE	B	1	19.264	39.105	1.314	0.00	0.00	6		CA	MET	B	1	27.955	47.832	4.826	0.00	0.00	6
	C	I LE	B	1	20.776	38.921	1.351	0.00	0.00	6		CB	MET	B	1	27.840	47.751	3.301	0.00	0.00	6
	C	I LE	B	1	18.579	37.928	2.019	0.00	0.00	6		C	MET	B	1	28.732	46.686	2.680	0.00	0.00	6
	C	I LE	B	1	18.555	36.654	1.206	0.00	0.00	6		SD	MET	B	1	28.571	46.613	0.886	0.00	0.00	1
	C	I LE	B	1	19.716	41.575	1.461	0.00	0.00	6		CE	MET	B	1	29.873	47.738	0.383	0.00	0.00	6
	O	I LE	B	1	20.702	41.937	2.103	0.00	0.00	8		C	MET	B	1	28.141	49.285	5.246	0.00	0.00	6

**FIG. 1-31B**



[illegible]

**FIG. 1-31C**

O	PRO	B	1	23.627	44.581	13.297	0.00	0.00	8
N	ARG	B	1	24.753	46.392	13.949	0.00	0.00	7
CA	ARG	B	1	23.680	46.909	14.785	0.00	0.00	6
CB	ARG	B	1	24.220	47.994	15.724	0.00	0.00	6
C	ARG	B	1	25.053	47.444	16.872	0.00	0.00	6
C	ARG	B	1	24.755	48.182	18.166	0.00	0.00	6
N	ARG	B	1	25.893	48.199	19.076	0.00	0.00	7
CZ	ARG	B	1	26.353	49.285	19.690	0.00	0.00	6
N	ARG	B	1	25.780	50.466	19.497	0.00	0.00	7
N	ARG	B	1	27.395	49.192	20.505	0.00	0.00	7
C	ARG	B	1	22.514	47.460	13.977	0.00	0.00	6
O	ARG	B	1	21.412	47.635	14.500	0.00	0.00	8
N	LYS	B	1	22.730	47.733	12.695	0.00	0.00	7
CA	LYS	B	1	21.703	48.240	11.804	0.00	0.00	6
CB	LYS	B	1	22.295	49.222	10.789	0.00	0.00	6
C	LYS	B	1	22.827	50.498	11.425	0.00	0.00	6
C	LYS	B	1	22.565	51.706	10.539	0.00	0.00	6
CE	LYS	B	1	21.724	52.748	11.258	0.00	0.00	6
NZ	LYS	B	1	20.929	53.572	10.304	0.00	0.00	7
C	LYS	B	1	20.981	47.102	11.086	0.00	0.00	6
O	LYS	B	1	20.040	47.343	10.330	0.00	0.00	8
N	ILE	B	1	21.424	45.867	11.305	0.00	0.00	7

N	VAL	B	1	16.502	37.077	9.381	0.00	0.00	7
CA	VAL	B	1	16.273	35.671	9.077	0.00	0.00	6
CB	VAL	B	1	16.761	34.775	10.235	0.00	0.00	6
C	VAL	B	1	16.528	33.300	9.955	0.00	0.00	6
C	VAL	B	1	18.237	35.028	10.508	0.00	0.00	6
C	VAL	B	1	14.848	35.319	8.695	0.00	0.00	6
O	VAL	B	1	14.578	34.863	7.578	0.00	0.00	8
N	PRO	B	1	13.874	35.543	9.572	0.00	0.00	7
C	PRO	B	1	14.098	36.089	10.939	0.00	0.00	6
CA	PRO	B	1	12.484	35.204	9.343	0.00	0.00	6
CB	PRO	B	1	11.775	35.569	10.644	0.00	0.00	6
C	PRO	B	1	12.827	35.760	11.666	0.00	0.00	6
C	PRO	B	1	11.804	35.891	8.174	0.00	0.00	6
O	PRO	B	1	10.742	35.457	7.712	0.00	0.00	8
N	SER	B	1	12.344	37.001	7.698	0.00	0.00	7
CA	SER	B	1	11.813	37.739	6.572	0.00	0.00	6
CB	SER	B	1	12.157	39.223	6.762	0.00	0.00	6
O	SER	B	1	13.534	39.457	6.544	0.00	0.00	8
C	SER	B	1	12.380	37.276	5.237	0.00	0.00	6
O	SER	B	1	11.814	37.593	4.187	0.00	0.00	8
N	THR	B	1	13.492	36.548	5.255	0.00	0.00	7
CA	THR	B	1	14.119	36.091	4.027	0.00	0.00	6

**FIG. 1-32A**





O	VAL	B	1	3.637	30.717	4.856	0.00	0.00	8
N	ALA	B	1	5.264	29.202	4.561	0.00	0.00	7
CA	ALA	B	1	4.540	28.115	5.214	0.00	0.00	6
CB	ALA	B	1	5.166	26.767	4.897	0.00	0.00	6
C	ALA	B	1	4.490	28.344	6.723	0.00	0.00	6
O	ALA	B	1	3.491	28.053	7.378	0.00	0.00	8
N	GLY	B	1	5.544	28.940	7.275	0.00	0.00	7
CA	GLY	B	1	5.559	29.332	8.678	0.00	0.00	6
C	GLY	B	1	4.428	30.316	8.970	0.00	0.00	6
O	GLY	B	1	3.660	30.100	9.905	0.00	0.00	8
N	HIS	B	1	4.297	31.369	8.172	0.00	0.00	7
CA	HIS	B	1	3.265	32.372	8.362	0.00	0.00	6
CB	HIS	B	1	3.500	33.598	7.458	0.00	0.00	6
C	HIS	B	1	4.431	34.570	8.124	0.00	0.00	6
C	HIS	B	1	4.275	35.318	9.242	0.00	0.00	6
N	HIS	B	1	5.706	34.815	7.668	0.00	0.00	7
CE	HIS	B	1	6.292	35.692	8.467	0.00	0.00	6
N	HIS	B	1	5.445	36.011	9.430	0.00	0.00	7
C	HIS	B	1	1.848	31.858	8.173	0.00	0.00	6
O	HIS	B	1	0.973	32.218	8.967	0.00	0.00	8
N	LEU	B	1	1.607	31.030	7.163	0.00	0.00	7
CA	LEU	B	1	0.266	30.503	6.932	0.00	0.00	6
CB	LEU	B	1	0.168	29.849	5.555	0.00	0.00	6

CA	GLY	B	1	-3.602	27.108	13.063	0.00	0.00	6
C	GLY	B	1	-3.408	25.731	12.443	0.00	0.00	6
O	GLY	B	1	-3.950	24.744	12.947	0.00	0.00	8
N	LEU	B	1	-2.623	25.649	11.371	0.00	0.00	7
CA	LEU	B	1	-2.343	24.371	10.718	0.00	0.00	6
CB	LEU	B	1	-1.965	24.563	9.253	0.00	0.00	6
C	LEU	B	1	-2.858	25.463	8.399	0.00	0.00	6
C	LEU	B	1	-2.224	25.720	7.038	0.00	0.00	6
C	LEU	B	1	-4.246	24.864	8.225	0.00	0.00	6
C	LEU	B	1	-1.230	23.648	11.474	0.00	0.00	6
O	LEU	B	1	-0.104	24.136	11.573	0.00	0.00	8
N	ARG	B	1	-1.566	22.508	12.067	0.00	0.00	7
CA	ARG	B	1	-0.631	21.762	12.899	0.00	0.00	6
CB	ARG	B	1	-1.276	21.448	14.255	0.00	0.00	6
C	ARG	B	1	-2.011	22.615	14.892	0.00	0.00	6
C	ARG	B	1	-1.894	22.647	16.405	0.00	0.00	6
N	ARG	B	1	-2.138	21.346	17.010	0.00	0.00	7
CZ	ARG	B	1	-1.376	20.762	17.925	0.00	0.00	6
N	ARG	B	1	-0.282	21.358	18.380	0.00	0.00	7
N	ARG	B	1	-1.706	19.564	18.391	0.00	0.00	7
C	ARG	B	1	-0.131	20.491	12.228	0.00	0.00	6
O	ARG	B	1	0.615	19.715	12.826	0.00	0.00	8
N	GLY	B	1	-0.521	20.281	10.975	0.00	0.00	7

**FIG. 1-33A**

[illegible]

**FIG. 1-33B**



C	ALA	B	1	14.257	24.163	-4.180	0.00	0.00	6
O	ALA	B	1	15.430	23.831	-4.015	0.00	0.00	8
N	THR	B	1	13.619	24.005	-5.336	0.00	0.00	7
CA	THR	B	1	14.295	23.435	-6.499	0.00	0.00	6
CB	THR	B	1	13.706	22.064	-6.879	0.00	0.00	6
O	THR	B	1	12.282	22.111	-6.725	0.00	0.00	8
C	THR	B	1	14.265	20.963	-5.992	0.00	0.00	6
C	THR	B	1	14.225	24.390	-7.684	0.00	0.00	6
O	THR	B	1	13.789	24.006	-8.770	0.00	0.00	8
N	ALA	B	1	14.611	25.645	-7.453	0.00	0.00	7
CA	ALA	B	1	14.614	26.639	-8.530	0.00	0.00	6
CB	ALA	B	1	15.804	26.381	-9.445	0.00	0.00	6
C	ALA	B	1	13.303	26.601	-9.297	0.00	0.00	6
O	ALA	B	1	12.228	26.596	-8.690	0.00	0.00	8
N	CYS	B	1	13.347	26.441	-10.615	0.00	0.00	7
CA	CYS	B	1	12.193	26.376	-11.482	0.00	0.00	6
CB	CYS	B	1	12.628	26.275	-12.957	0.00	0.00	6
SG	CYS	B	1	14.176	27.109	-13.348	0.00	0.00	1
C	CYS	B	1	11.226	25.225	-11.252	0.00	0.00	6
O	CYS	B	1	10.137	25.253	-11.841	0.00	0.00	8
N	THR	B	1	11.590	24.199	-10.504	0.00	0.00	7
CA	THR	B	1	10.719	23.048	-10.288	0.00	0.00	6

CB	ILE	B	1	1.889	20.822	-6.382	0.00	0.00	6
C	ILE	B	1	0.616	20.091	-6.787	0.00	0.00	6
C	ILE	B	1	1.623	22.325	-6.258	0.00	0.00	6
C	ILE	B	1	1.353	23.023	-7.570	0.00	0.00	6
C	ILE	B	1	2.446	18.758	-5.061	0.00	0.00	6
O	ILE	B	1	1.580	18.154	-4.427	0.00	0.00	8
N	GLY	B	1	3.384	18.133	-5.762	0.00	0.00	7
CA	GLY	B	1	3.472	16.684	-5.812	0.00	0.00	6
C	GLY	B	1	3.809	16.032	-4.479	0.00	0.00	6
O	GLY	B	1	3.271	14.959	-4.179	0.00	0.00	8
N	HIS	B	1	4.669	16.644	-3.659	0.00	0.00	7
CA	HIS	B	1	5.026	16.030	-2.374	0.00	0.00	6
CB	HIS	B	1	6.437	16.407	-1.924	0.00	0.00	6
C	HIS	B	1	7.414	15.486	-2.612	0.00	0.00	6
C	HIS	B	1	7.712	14.188	-2.381	0.00	0.00	6
N	HIS	B	1	8.157	15.865	-3.705	0.00	0.00	7
CE	HIS	B	1	8.893	14.846	-4.108	0.00	0.00	6
N	HIS	B	1	8.641	13.816	-3.321	0.00	0.00	7
C	HIS	B	1	3.927	16.250	-1.352	0.00	0.00	6
O	HIS	B	1	3.717	15.434	-0.451	0.00	0.00	8
N	ALA	B	1	3.120	17.291	-1.551	0.00	0.00	7
CA	ALA	B	1	1.950	17.523	-0.711	0.00	0.00	6

**FIG. 1-34A**







CB	TYR	B	1	2.014	8.854	2.943	0.00	0.00	6
C	TYR	B	1	2.850	7.925	3.794	0.00	0.00	6
C	TYR	B	1	3.636	6.939	3.212	0.00	0.00	6
CE	TYR	B	1	4.401	6.086	3.986	0.00	0.00	6
C	TYR	B	1	2.852	8.034	5.177	0.00	0.00	6
CE	TYR	B	1	3.610	7.186	5.958	0.00	0.00	6
CZ	TYR	B	1	4.384	6.216	5.358	0.00	0.00	6
O	TYR	B	1	5.142	5.374	6.138	0.00	0.00	8
C	TYR	B	1	-0.198	8.250	3.937	0.00	0.00	6
O	TYR	B	1	-0.104	7.256	4.662	0.00	0.00	8
N	GLY	B	1	-0.963	9.293	4.248	0.00	0.00	7
CA	GLY	B	1	-1.773	9.308	5.455	0.00	0.00	6
C	GLY	B	1	-1.314	10.320	6.490	0.00	0.00	6
O	GLY	B	1	-1.960	10.471	7.533	0.00	0.00	8
N	ASP	B	1	-0.278	11.098	6.180	0.00	0.00	7
CA	ASP	B	1	0.254	12.078	7.116	0.00	0.00	6
CB	ASP	B	1	1.692	12.465	6.736	0.00	0.00	6
C	ASP	B	1	2.678	11.416	7.227	0.00	0.00	6
O	ASP	B	1	3.710	11.204	6.560	0.00	0.00	8
O	ASP	B	1	2.400	10.811	8.284	0.00	0.00	8
C	ASP	B	1	-0.599	13.330	7.234	0.00	0.00	6
O	ASP	B	1	-0.518	14.047	8.234	0.00	0.00	8

C	GLY	B	1	3.936	26.714	-3.879	0.00	0.00	6
O	GLY	B	1	4.803	26.194	-3.181	0.00	0.00	8
N	GLY	B	1	4.122	27.849	-4.543	0.00	0.00	7
CA	GLY	B	1	5.387	28.564	-4.497	0.00	0.00	6
C	GLY	B	1	5.124	30.062	-4.611	0.00	0.00	6
O	GLY	B	1	4.054	30.504	-5.026	0.00	0.00	8
N	ALA	B	1	6.124	30.827	-4.211	0.00	0.00	7
CA	ALA	B	1	6.071	32.279	-4.285	0.00	0.00	6
CB	ALA	B	1	5.563	32.894	-3.001	0.00	0.00	6
C	ALA	B	1	7.484	32.761	-4.618	0.00	0.00	6
O	ALA	B	1	8.460	32.155	-4.182	0.00	0.00	8
N	GLU	B	1	7.573	33.801	-5.429	0.00	0.00	7
CA	GLU	B	1	8.863	34.352	-5.816	0.00	0.00	6
CB	GLU	B	1	9.419	33.641	-7.049	0.00	0.00	6
C	GLU	B	1	10.909	33.815	-7.291	0.00	0.00	6
C	GLU	B	1	11.720	32.733	-6.598	0.00	0.00	6
O	GLU	B	1	11.478	31.534	-6.865	0.00	0.00	8
O	GLU	B	1	12.584	33.086	-5.773	0.00	0.00	8
C	GLU	B	1	8.715	35.844	-6.094	0.00	0.00	6
O	GLU	B	1	7.669	36.320	-6.521	0.00	0.00	8
N	LYS	B	1	9.780	36.575	-5.833	0.00	0.00	7
CA	LYS	B	1	9.876	37.996	-6.134	0.00	0.00	6

**FIG. 1-35A**

N	ALA	B	1	-1.408	13.603	6.218	0.00	0.00	7
CA	ALA	B	1	-2.282	14.768	6.227	0.00	0.00	6
CB	ALA	B	1	-1.545	15.978	5.671	0.00	0.00	6
C	ALA	B	1	-3.538	14.484	5.410	0.00	0.00	6
O	ALA	B	1	-3.555	13.544	4.613	0.00	0.00	8
N	ASP	B	1	-4.573	15.288	5.622	0.00	0.00	7
CA	ASP	B	1	-5.808	15.128	4.857	0.00	0.00	6
CB	ASP	B	1	-7.045	15.068	5.746	0.00	0.00	6
C	ASP	B	1	-7.073	13.809	6.598	0.00	0.00	6
O	ASP	B	1	-7.526	13.894	7.758	0.00	0.00	8
O	ASP	B	1	-6.629	12.750	6.106	0.00	0.00	8
C	ASP	B	1	-5.893	16.279	3.854	0.00	0.00	6
O	ASP	B	1	-6.203	16.091	2.684	0.00	0.00	8
N	VAL	B	1	-5.540	17.471	4.321	0.00	0.00	7
CA	VAL	B	1	-5.493	18.672	3.508	0.00	0.00	6
CB	VAL	B	1	-6.459	19.763	4.011	0.00	0.00	6
C	VAL	B	1	-6.406	20.998	3.114	0.00	0.00	6
C	VAL	B	1	-7.895	19.274	4.108	0.00	0.00	6
C	VAL	B	1	-4.086	19.272	3.518	0.00	0.00	6
O	VAL	B	1	-3.427	19.305	4.555	0.00	0.00	8
N	MET	B	1	-3.639	19.782	2.378	0.00	0.00	7

**FIG. 1-35B**



C	GLY	B	1	18.231	39.294	-10.841	0.00	0.00	6
O	GLY	B	1	18.482	38.368	-11.616	0.00	0.00	8
N	VAL	B	1	18.012	40.540	-11.257	0.00	0.00	7
CA	VAL	B	1	18.114	40.877	-12.680	0.00	0.00	6
CB	VAL	B	1	17.522	42.254	-13.000	0.00	0.00	6
C	VAL	B	1	17.585	42.548	-14.492	0.00	0.00	6
C	VAL	B	1	16.080	42.340	-12.516	0.00	0.00	6
C	VAL	B	1	19.580	40.788	-13.100	0.00	0.00	6
O	VAL	B	1	19.934	40.087	-14.046	0.00	0.00	8
N	GLY	B	2	20.452	41.426	-12.326	0.00	0.00	7
CA	GLY	B	2	21.880	41.395	-12.580	0.00	0.00	6
C	GLY	B	2	22.468	39.993	-12.607	0.00	0.00	6
O	GLY	B	2	23.247	39.675	-13.505	0.00	0.00	8
N	GLY	B	2	22.151	39.157	-11.627	0.00	0.00	7
CA	GLY	B	2	22.680	37.817	-11.495	0.00	0.00	6
C	GLY	B	2	22.380	36.909	-12.672	0.00	0.00	6
O	GLY	B	2	23.254	36.212	-13.187	0.00	0.00	8
N	PHE	B	2	21.128	36.914	-13.116	0.00	0.00	7
CA	PHE	B	2	20.705	36.129	-14.269	0.00	0.00	6
CB	PHE	B	2	19.188	35.986	-14.314	0.00	0.00	6
C	PHE	B	2	18.629	34.898	-13.445	0.00	0.00	6
C	PHE	B	2	17.786	35.206	-12.390	0.00	0.00	6

C	LEU	B	2	17.844	37.339	-21.197	0.00	0.00	6
O	LEU	B	2	18.868	37.677	-21.784	0.00	0.00	8
N	SER	B	2	16.623	37.549	-21.687	0.00	0.00	7
CA	SER	B	2	16.421	38.239	-22.955	0.00	0.00	6
CB	SER	B	2	14.966	38.166	-23.409	0.00	0.00	6
O	SER	B	2	14.690	39.185	-24.358	0.00	0.00	8
C	SER	B	2	16.826	39.705	-22.784	0.00	0.00	6
O	SER	B	2	16.722	40.242	-21.680	0.00	0.00	8
N	THR	B	2	17.273	40.344	-23.859	0.00	0.00	7
CA	THR	B	2	17.738	41.737	-23.762	0.00	0.00	6
CB	THR	B	2	19.260	41.759	-23.962	0.00	0.00	6
O	THR	B	2	19.868	41.092	-22.832	0.00	0.00	8
C	THR	B	2	19.889	43.137	-24.035	0.00	0.00	6
C	THR	B	2	16.962	42.631	-24.708	0.00	0.00	6
O	THR	B	2	17.285	43.792	-24.973	0.00	0.00	8
N	ARG	B	2	15.782	42.175	-25.133	0.00	0.00	7
CA	ARG	B	2	14.924	42.914	-26.051	0.00	0.00	6
CB	ARG	B	2	13.923	41.938	-26.690	0.00	0.00	6
C	ARG	B	2	13.305	42.435	-27.985	0.00	0.00	6
C	ARG	B	2	12.311	41.433	-28.553	0.00	0.00	6
N	ARG	B	2	12.906	40.609	-29.599	0.00	0.00	7
CZ	ARG	B	2	13.523	39.451	-29.399	0.00	0.00	6

**FIG. 1-36A**







C	GLN	B	2	6.387	41.211	-25.635	0.00	0.00	6
O	GLN	B	2	5.582	40.281	-25.739	0.00	0.00	8
N	ALA	B	2	7.407	41.356	-26.466	0.00	0.00	7
CA	ALA	B	2	7.686	40.389	-27.521	0.00	0.00	6
CB	ALA	B	2	7.796	41.094	-28.865	0.00	0.00	6
C	ALA	B	2	8.973	39.631	-27.213	0.00	0.00	6
O	ALA	B	2	9.383	38.727	-27.940	0.00	0.00	8
N	ALA	B	2	9.608	40.009	-26.111	0.00	0.00	7
CA	ALA	B	2	10.855	39.404	-25.669	0.00	0.00	6
CB	ALA	B	2	11.386	40.154	-24.455	0.00	0.00	6
C	ALA	B	2	10.695	37.924	-25.350	0.00	0.00	6
O	ALA	B	2	11.503	37.104	-25.790	0.00	0.00	8
N	SER	B	2	9.673	37.586	-24.574	0.00	0.00	7
CA	SER	B	2	9.427	36.187	-24.222	0.00	0.00	6
CB	SER	B	2	8.587	36.099	-22.951	0.00	0.00	6
O	SER	B	2	8.334	34.748	-22.607	0.00	0.00	8
C	SER	B	2	8.745	35.507	-25.402	0.00	0.00	6
O	SER	B	2	7.552	35.705	-25.621	0.00	0.00	8
N	ARG	B	2	9.501	34.722	-26.158	0.00	0.00	7
CA	ARG	B	2	8.972	34.053	-27.343	0.00	0.00	6
CB	ARG	B	2	9.340	34.866	-28.594	0.00	0.00	6
C	ARG	B	2	10.801	35.257	-28.718	0.00	0.00	6

NZ	LYS	B	2	15.416	35.744	-37.419	0.00	0.00	7
C	LYS	B	2	14.662	32.808	-33.361	0.00	0.00	6
O	LYS	B	2	15.883	32.672	-33.235	0.00	0.00	8
N	GLU	B	2	14.035	33.916	-32.989	0.00	0.00	7
CA	GLU	B	2	14.726	35.061	-32.424	0.00	0.00	6
CB	GLU	B	2	13.994	36.350	-32.810	0.00	0.00	6
C	GLU	B	2	13.999	36.700	-34.291	0.00	0.00	6
C	GLU	B	2	13.184	37.968	-34.508	0.00	0.00	6
O	GLU	B	2	13.724	39.057	-34.221	0.00	0.00	8
O	GLU	B	2	12.017	37.858	-34.934	0.00	0.00	8
C	GLU	B	2	14.885	35.037	-30.910	0.00	0.00	6
O	GLU	B	2	15.305	36.051	-30.338	0.00	0.00	8
N	ARG	B	2	14.572	33.939	-30.240	0.00	0.00	7
CA	ARG	B	2	14.764	33.797	-28.809	0.00	0.00	6
CB	ARG	B	2	14.709	32.328	-28.382	0.00	0.00	6
C	ARG	B	2	13.360	31.659	-28.338	0.00	0.00	6
C	ARG	B	2	13.481	30.147	-28.281	0.00	0.00	6
N	ARG	B	2	14.578	29.612	-29.063	0.00	0.00	7
CZ	ARG	B	2	14.646	28.397	-29.592	0.00	0.00	6
N	ARG	B	2	13.659	27.524	-29.440	0.00	0.00	7
N	ARG	B	2	15.720	28.042	-30.289	0.00	0.00	7
C	ARG	B	2	16.145	34.280	-28.362	0.00	0.00	6

**FIG. 1-37A**

[illegible]

**FIG. 1-37B**



O	GLY	B	2	8.864	36.154	-11.456	0.00	0.00	8
N	ASP	B	2	7.357	37.812	-11.419	0.00	0.00	7
CA	ASP	B	2	7.049	37.681	-10.007	0.00	0.00	6
CB	ASP	B	2	7.131	39.013	-9.261	0.00	0.00	6
C	ASP	B	2	8.433	39.754	-9.450	0.00	0.00	6
O	ASP	B	2	9.502	39.115	-9.377	0.00	0.00	8
O	ASP	B	2	8.386	40.980	-9.676	0.00	0.00	8
C	ASP	B	2	5.629	37.151	-9.804	0.00	0.00	6
O	ASP	B	2	4.764	37.359	-10.654	0.00	0.00	8
N	GLY	B	2	5.394	36.540	-8.644	0.00	0.00	7
CA	GLY	B	2	4.060	36.050	-8.336	0.00	0.00	6
C	GLY	B	2	4.049	34.883	-7.363	0.00	0.00	6
O	GLY	B	2	5.018	34.582	-6.671	0.00	0.00	8
N	ALA	B	2	2.897	34.226	-7.305	0.00	0.00	7
CA	ALA	B	2	2.672	33.116	-6.393	0.00	0.00	6
CB	ALA	B	2	2.668	33.596	-4.948	0.00	0.00	6
C	ALA	B	2	1.336	32.447	-6.706	0.00	0.00	6
O	ALA	B	2	0.329	33.123	-6.890	0.00	0.00	8
N	GLY	B	2	1.363	31.129	-6.779	0.00	0.00	7
CA	GLY	B	2	0.163	30.338	-7.029	0.00	0.00	6

CB	GLU	B	2	-7.982	12.690	1.450	0.00	0.00	6
C	GLU	B	2	-8.173	11.195	1.233	0.00	0.00	6
C	GLU	B	2	-9.627	10.801	1.445	0.00	0.00	6
O	GLU	B	2	-10.283	11.423	2.308	0.00	0.00	8
O	GLU	B	2	-10.094	9.890	0.734	0.00	0.00	8
C	GLU	B	2	-9.584	13.491	-0.338	0.00	0.00	6
O	GLU	B	2	-10.468	14.184	0.159	0.00	0.00	8
N	TYR	B	2	-9.813	12.671	-1.355	0.00	0.00	7
CA	TYR	B	2	-11.109	12.554	-1.999	0.00	0.00	6
CB	TYR	B	2	-11.091	11.397	-3.007	0.00	0.00	6
C	TYR	B	2	-12.367	11.296	-3.815	0.00	0.00	6
C	TYR	B	2	-12.773	12.324	-4.653	0.00	0.00	6
CE	TYR	B	2	-13.942	12.226	-5.385	0.00	0.00	6
C	TYR	B	2	-13.166	10.165	-3.726	0.00	0.00	6
CE	TYR	B	2	-14.337	10.059	-4.453	0.00	0.00	6
CZ	TYR	B	2	-14.718	11.092	-5.281	0.00	0.00	6
O	TYR	B	2	-15.882	10.989	-6.005	0.00	0.00	8
C	TYR	B	2	-12.290	12.410	-1.056	0.00	0.00	6
O	TYR	B	2	-13.194	13.253	-1.067	0.00	0.00	8
N	GLU	B	2	-12.307	11.371	-0.230	0.00	0.00	7

**FIG. 1-38A**

[illegible]

**FIG. 1-38B**



C	ARG	B	2	-16.629	18.877	5.361	0.00	0.00	6
C	ARG	B	2	-15.223	18.495	5.797	0.00	0.00	6
N	ARG	B	2	-15.208	17.305	6.639	0.00	0.00	7
CZ	ARG	B	2	-14.361	17.075	7.633	0.00	0.00	6
N	ARG	B	2	-13.421	17.958	7.948	0.00	0.00	7
N	ARG	B	2	-14.446	15.947	8.329	0.00	0.00	7
C	ARG	B	2	-18.598	18.849	2.129	0.00	0.00	6
O	ARG	B	2	-19.177	19.924	2.276	0.00	0.00	8
N	GLY	B	2	-18.496	18.262	0.942	0.00	0.00	7
CA	GLY	B	2	-19.076	18.799	-0.271	0.00	0.00	6
C	GLY	B	2	-18.336	19.987	-0.860	0.00	0.00	6
O	GLY	B	2	-18.940	21.015	-1.171	0.00	0.00	8
N	ALA	B	2	-17.031	19.848	-1.051	0.00	0.00	7
CA	ALA	B	2	-16.202	20.919	-1.579	0.00	0.00	6
CB	ALA	B	2	-14.759	20.689	-1.128	0.00	0.00	6
C	ALA	B	2	-16.233	21.053	-3.095	0.00	0.00	6
O	ALA	B	2	-16.500	20.108	-3.829	0.00	0.00	8
N	LYS	B	2	-15.861	22.242	-3.565	0.00	0.00	7
CA	LYS	B	2	-15.628	22.494	-4.982	0.00	0.00	6
C	LEU	B	2	-1.005	16.692	-6.980	0.00	0.00	6
C	LEU	B	2	-0.754	14.976	-8.775	0.00	0.00	6
C	LEU	B	2	-3.657	13.429	-9.133	0.00	0.00	6
O	LEU	B	2	-3.958	12.694	-8.188	0.00	0.00	8
N	VAL	B	2	-3.337	12.963	-10.335	0.00	0.00	7
CA	VAL	B	2	-3.267	11.527	-10.582	0.00	0.00	6
CB	VAL	B	2	-4.193	11.094	-11.743	0.00	0.00	6
C	VAL	B	2	-5.657	11.300	-11.386	0.00	0.00	6
C	VAL	B	2	-3.845	11.841	-13.021	0.00	0.00	6
C	VAL	B	2	-1.870	11.009	-10.886	0.00	0.00	6
O	VAL	B	2	-1.669	9.791	-10.859	0.00	0.00	8
N	GLY	B	2	-0.927	11.891	-11.202	0.00	0.00	7
CA	GLY	B	2	0.427	11.452	-11.517	0.00	0.00	6
C	GLY	B	2	1.485	12.468	-11.115	0.00	0.00	6
O	GLY	B	2	1.280	13.678	-11.198	0.00	0.00	8
N	PHE	B	2	2.636	11.965	-10.676	0.00	0.00	7
CA	PHE	B	2	3.762	12.806	-10.292	0.00	0.00	6
CB	PHE	B	2	3.755	13.148	-8.806	0.00	0.00	6
C	PHE	B	2	4.902	13.995	-8.332	0.00	0.00	6

**FIG. 1-39A**







CA	TYR	B	2	24.503	16.907	-17.311	0.00	0.00	6
CB	TYR	B	2	23.451	17.038	-18.431	0.00	0.00	6
C	TYR	B	2	24.048	17.513	-19.738	0.00	0.00	6
C	TYR	B	2	24.764	16.646	-20.552	0.00	0.00	6
CE	TYR	B	2	25.328	17.085	-21.735	0.00	0.00	6
C	TYR	B	2	23.920	18.836	-20.138	0.00	0.00	6
CE	TYR	B	2	24.481	19.285	-21.317	0.00	0.00	6
CZ	TYR	B	2	25.184	18.403	-22.110	0.00	0.00	6
O	TYR	B	2	25.745	18.844	-23.288	0.00	0.00	8
C	TYR	B	2	25.213	18.225	-17.058	0.00	0.00	6
O	TYR	B	2	26.443	18.260	-16.980	0.00	0.00	8
N	HIS	B	2	24.468	19.317	-16.925	0.00	0.00	7
CA	HIS	B	2	25.063	20.628	-16.677	0.00	0.00	6
CB	HIS	B	2	25.120	21.431	-17.973	0.00	0.00	6
C	HIS	B	2	25.949	22.675	-17.927	0.00	0.00	6
C	HIS	B	2	27.279	22.868	-18.087	0.00	0.00	6
N	HIS	B	2	25.406	23.923	-17.701	0.00	0.00	7
CE	HIS	B	2	26.363	24.831	-17.719	0.00	0.00	6
N	HIS	B	2	27.510	24.217	-17.952	0.00	0.00	7
C	HIS	B	2	24.288	21.375	-15.598	0.00	0.00	6
O	HIS	B	2	23.085	21.157	-15.436	0.00	0.00	8
N	MET	B	2	24.946	22.292	-14.889	0.00	0.00	7

O	GLU	B	2	17.914	17.862	-27.146	0.00	0.00	8
N	ASN	B	2	19.270	16.400	-26.211	0.00	0.00	7
CA	ASN	B	2	18.435	15.232	-26.207	0.00	0.00	6
CB	ASN	B	2	19.172	14.173	-25.349	0.00	0.00	6
C	ASN	B	2	18.845	12.748	-25.717	0.00	0.00	6
O	ASN	B	2	19.753	11.936	-25.906	0.00	0.00	8
N	ASN	B	2	17.563	12.424	-25.817	0.00	0.00	7
C	ASN	B	2	17.071	15.424	-25.550	0.00	0.00	6
O	ASN	B	2	16.066	14.871	-25.996	0.00	0.00	8
N	GLY	B	2	17.065	16.049	-24.372	0.00	0.00	7
CA	GLY	B	2	15.866	16.222	-23.566	0.00	0.00	6
C	GLY	B	2	15.598	14.984	-22.712	0.00	0.00	6
O	GLY	B	2	14.492	14.758	-22.223	0.00	0.00	8
N	ALA	B	2	16.622	14.173	-22.501	0.00	0.00	7
CA	ALA	B	2	16.575	12.927	-21.771	0.00	0.00	6
CB	ALA	B	2	17.997	12.361	-21.662	0.00	0.00	6
C	ALA	B	2	15.955	12.959	-20.385	0.00	0.00	6
O	ALA	B	2	15.249	12.014	-20.012	0.00	0.00	8
N	GLY	B	2	16.284	13.950	-19.564	0.00	0.00	7
CA	GLY	B	2	15.732	14.032	-18.215	0.00	0.00	6
C	GLY	B	2	14.264	14.437	-18.254	0.00	0.00	6
O	GLY	B	2	13.456	13.967	-17.452	0.00	0.00	8

**FIG. 1-40A**

[illegible]

**FIG. 1-40B**



C	ASN	B	2	6.197	8.998	-14.279	0.00	0.00	6
O	ASN	B	2	5.503	8.220	-13.619	0.00	0.00	8
N	ALA	B	2	5.777	10.216	-14.603	0.00	0.00	7
CA	ALA	B	2	4.454	10.699	-14.218	0.00	0.00	6
CB	ALA	B	2	4.306	12.172	-14.556	0.00	0.00	6
C	ALA	B	2	3.368	9.877	-14.905	0.00	0.00	6
O	ALA	B	2	2.352	9.517	-14.309	0.00	0.00	8
N	LEU	B	2	3.579	9.576	-16.183	0.00	0.00	7
CA	LEU	B	2	2.697	8.712	-16.953	0.00	0.00	6
CB	LEU	B	2	3.249	8.513	-18.366	0.00	0.00	6
C	LEU	B	2	3.101	9.673	-19.350	0.00	0.00	6
C	LEU	B	2	3.754	9.327	-20.681	0.00	0.00	6
C	LEU	B	2	1.639	10.039	-19.560	0.00	0.00	6
C	LEU	B	2	2.529	7.358	-16.271	0.00	0.00	6
O	LEU	B	2	1.414	6.913	-16.001	0.00	0.00	8
N	ARG	B	2	3.649	6.713	-15.949	0.00	0.00	7
CA	ARG	B	2	3.632	5.420	-15.266	0.00	0.00	6
CB	ARG	B	2	5.055	4.885	-15.124	0.00	0.00	6
C	ARG	B	2	5.269	3.835	-14.048	0.00	0.00	6
C	ARG	B	2	6.689	3.295	-14.066	0.00	0.00	6

O	ALA	B	2	-0.518	11.392	-24.609	0.00	0.00	8
N	SER	B	2	-1.137	9.337	-25.190	0.00	0.00	7
CA	SER	B	2	-2.220	9.753	-26.061	0.00	0.00	6
CB	SER	B	2	-2.484	8.658	-27.106	0.00	0.00	6
O	SER	B	2	-3.091	7.533	-26.492	0.00	0.00	8
C	SER	B	2	-3.518	10.076	-25.337	0.00	0.00	6
O	SER	B	2	-4.542	10.359	-25.965	0.00	0.00	8
N	GLN	B	2	-3.509	10.047	-24.013	0.00	0.00	7
CA	GLN	B	2	-4.668	10.363	-23.192	0.00	0.00	6
CB	GLN	B	2	-4.827	9.353	-22.058	0.00	0.00	6
C	GLN	B	2	-5.411	8.026	-22.514	0.00	0.00	6
C	GLN	B	2	-5.194	6.897	-21.531	0.00	0.00	6
O	GLN	B	2	-5.872	6.804	-20.506	0.00	0.00	8
N	GLN	B	2	-4.244	6.019	-21.837	0.00	0.00	7
C	GLN	B	2	-4.523	11.789	-22.658	0.00	0.00	6
O	GLN	B	2	-5.433	12.355	-22.059	0.00	0.00	8
N	ILE	B	2	-3.356	12.376	-22.904	0.00	0.00	7
CA	ILE	B	2	-3.062	13.745	-22.523	0.00	0.00	6
CB	ILE	B	2	-1.568	13.957	-22.207	0.00	0.00	6
C	ILE	B	2	-1.273	15.420	-21.897	0.00	0.00	6

**FIG. 1-41A**

[illegible]

**FIG. 1-41B**



C	HIS	B	3	10.390	25.210	-16.758	0.00	0.00	6
N	HIS	B	3	11.903	24.910	-18.306	0.00	0.00	7
CE	HIS	B	3	12.452	25.651	-17.361	0.00	0.00	6
N	HIS	B	3	11.555	25.849	-16.411	0.00	0.00	7
C	HIS	B	3	8.713	25.840	-20.012	0.00	0.00	6
O	HIS	B	3	8.552	26.963	-19.544	0.00	0.00	8
N	GLY	B	3	8.959	25.668	-21.304	0.00	0.00	7
CA	GLY	B	3	9.110	26.699	-22.298	0.00	0.00	6
C	GLY	B	3	9.520	28.073	-21.817	0.00	0.00	6
O	GLY	B	3	8.705	29.001	-21.787	0.00	0.00	8
N	THR	B	3	10.795	28.256	-21.485	0.00	0.00	7
CA	THR	B	3	11.269	29.531	-20.965	0.00	0.00	6
CB	THR	B	3	12.393	29.318	-19.926	0.00	0.00	6
O	THR	B	3	13.417	28.495	-20.489	0.00	0.00	8
C	THR	B	3	11.814	28.661	-18.686	0.00	0.00	6
C	THR	B	3	11.749	30.530	-21.994	0.00	0.00	6
O	THR	B	3	11.989	31.682	-21.621	0.00	0.00	8
N	SER	B	3	11.871	30.151	-23.253	0.00	0.00	7
CA	SER	B	3	12.296	31.048	-24.316	0.00	0.00	6
CB	SER	B	3	11.700	32.449	-24.195	0.00	0.00	6
O	SER	B	3	11.945	33.196	-25.377	0.00	0.00	8
C	SER	B	3	13.817	31.113	-24.425	0.00	0.00	6

CA	ALA	B	3	15.321	19.999	-25.558	0.00	0.00	6
CB	ALA	B	3	16.151	20.211	-24.301	0.00	0.00	6
C	ALA	B	3	13.924	19.512	-25.199	0.00	0.00	6
O	ALA	B	3	13.580	18.357	-25.449	0.00	0.00	8
N	GLU	B	3	13.106	20.401	-24.642	0.00	0.00	7
CA	GLU	B	3	11.734	20.071	-24.292	0.00	0.00	6
CB	GLU	B	3	11.017	21.263	-23.650	0.00	0.00	6
C	GLU	B	3	9.583	20.941	-23.264	0.00	0.00	6
C	GLU	B	3	8.946	21.951	-22.340	0.00	0.00	6
O	GLU	B	3	9.409	23.108	-22.269	0.00	0.00	8
O	GLU	B	3	7.952	21.571	-21.682	0.00	0.00	8
C	GLU	B	3	10.956	19.598	-25.515	0.00	0.00	6
O	GLU	B	3	10.335	18.535	-25.473	0.00	0.00	8
N	ALA	B	3	11.030	20.340	-26.616	0.00	0.00	7
CA	ALA	B	3	10.418	19.917	-27.874	0.00	0.00	6
CB	ALA	B	3	10.878	20.817	-29.012	0.00	0.00	6
C	ALA	B	3	10.765	18.460	-28.169	0.00	0.00	6
O	ALA	B	3	9.903	17.589	-28.253	0.00	0.00	8
N	GLN	B	3	12.057	18.168	-28.245	0.00	0.00	7
CA	GLN	B	3	12.595	16.840	-28.467	0.00	0.00	6
CB	GLN	B	3	14.128	16.919	-28.418	0.00	0.00	6
C	GLN	B	3	14.837	15.647	-28.840	0.00	0.00	6

**FIG. 1-42A**



	O	SER	B	3	14.407	32.108	-24.845	0.00	0.00	8	C	GLN	B	3	14.676	15.342	-30.316	0.00	0.00	6
	N	THR	B	3	14.456	30.008	-24.054	0.00	0.00	7	O	GLN	B	3	15.369	15.914	-31.156	0.00	0.00	8
	CA	THR	B	3	15.905	29.885	-24.172	0.00	0.00	6	N	GLN	B	3	13.752	14.439	-30.630	0.00	0.00	7
	CB	THR	B	3	16.565	29.275	-22.928	0.00	0.00	6	C	GLN	B	3	12.106	15.797	-27.473	0.00	0.00	6
	O	THR	B	3	15.830	28.108	-22.530	0.00	0.00	8	O	GLN	B	3	11.875	14.642	-27.844	0.00	0.00	8
	C	THR	B	3	16.593	30.277	-21.786	0.00	0.00	6	N	ALA	B	3	11.921	16.171	-26.211	0.00	0.00	7
	C	THR	B	3	16.187	28.984	-25.372	0.00	0.00	6	CA	ALA	B	3	11.429	15.277	-25.178	0.00	0.00	6
	O	THR	B	3	15.513	27.968	-25.556	0.00	0.00	8	CB	ALA	B	3	11.680	15.890	-23.803	0.00	0.00	6
	N	PRO	B	3	17.140	29.376	-26.198	0.00	0.00	7	C	ALA	B	3	9.950	14.942	-25.329	0.00	0.00	6
	C	PRO	B	3	17.984	30.585	-26.036	0.00	0.00	6	O	ALA	B	3	9.512	13.883	-24.874	0.00	0.00	8
	CA	PRO	B	3	17.543	28.578	-27.343	0.00	0.00	6	N	VAL	B	3	9.171	15.827	-25.938	0.00	0.00	7
	CB	PRO	B	3	18.871	29.194	-27.764	0.00	0.00	6	CA	VAL	B	3	7.748	15.592	-26.168	0.00	0.00	6
	C	PRO	B	3	18.799	30.609	-27.303	0.00	0.00	6	CB	VAL	B	3	6.977	16.904	-26.378	0.00	0.00	6
	C	PRO	B	3	17.675	27.110	-26.977	0.00	0.00	6	C	VAL	B	3	5.548	16.665	-26.846	0.00	0.00	6
	O	PRO	B	3	16.843	26.287	-27.366	0.00	0.00	8	C	VAL	B	3	6.973	17.714	-25.087	0.00	0.00	6
	N	ALA	B	3	18.660	26.778	-26.149	0.00	0.00	7	C	VAL	B	3	7.563	14.663	-27.364	0.00	0.00	6
	CA	ALA	B	3	18.923	25.406	-25.745	0.00	0.00	6	O	VAL	B	3	6.690	13.795	-27.365	0.00	0.00	8
	CB	ALA	B	3	20..34	25.368	-24.855	0.00	0.00	6	N	LYS	B	3	8.449	14.789	-28.349	0.00	0.00	7
	C	ALA	B	3	17.765	24.708	-25.053	0.00	0.00	6	CA	LYS	B	3	8.452	13.883	-29.494	0.00	0.00	6
	O	ALA	B	3	17.474	23.546	-25.367	0.00	0.00	8	CB	LYS	B	3	9.497	14.318	-30.523	0.00	0.00	6
	N	GLY	B	3	17.115	25.356	-24.096	0.00	0.00	7	C	LYS	B	3	9.016	15.457	-31.412	0.00	0.00	6

**FIG. 1-42B**



CA	PHE	B	3	4.069	11.077	-27.288	0.00	0.00	6
CB	PHE	B	3	3.425	12.453	-27.452	0.00	0.00	6
C	PHE	B	3	3.089	13.122	-26.147	0.00	0.00	6
C	PHE	B	3	4.076	13.702	-25.370	0.00	0.00	6
C	PHE	B	3	1.779	13.179	-25.702	0.00	0.00	6
CE	PHE	B	3	3.770	14.318	-24.173	0.00	0.00	6
CE	PHE	B	3	1.464	13.796	-24.507	0.00	0.00	6
CZ	PHE	B	3	2.461	14.366	-23.740	0.00	0.00	6
C	PHE	B	3	4.151	10.329	-28.610	0.00	0.00	6
O	PHE	B	3	3.231	9.594	-28.973	0.00	0.00	8
N	GLY	B	3	5.262	10.477	-29.320	0.00	0.00	7
CA	GLY	B	3	5.513	9.754	-30.551	0.00	0.00	6
C	GLY	B	3	4.558	10.072	-31.687	0.00	0.00	6
O	GLY	B	3	4.725	11.071	-32.388	0.00	0.00	8
N	GLU	B	3	3.556	9.216	-31.888	0.00	0.00	7
CA	GLU	B	3	2.598	9.393	-32.975	0.00	0.00	6
CB	GLU	B	3	2.032	8.053	-33.443	0.00	0.00	6
C	GLU	B	3	2.877	7.373	-34.517	0.00	0.00	6
C	GLU	B	3	3.606	6.164	-33.959	0.00	0.00	6
O	GLU	B	3	4.772	6.319	-33.536	0.00	0.00	8

O	LEU	B	3	-0.553	20.670	-25.402	0.00	0.00	8
N	VAL	B	3	0.701	21.702	-26.934	0.00	0.00	7
CA	VAL	B	3	1.738	22.123	-26.006	0.00	0.00	6
CB	VAL	B	3	3.106	21.485	-26.333	0.00	0.00	6
C	VAL	B	3	4.155	21.927	-25.318	0.00	0.00	6
C	VAL	B	3	3.050	19.970	-26.391	0.00	0.00	6
C	VAL	B	3	1.924	23.638	-26.057	0.00	0.00	6
O	VAL	B	3	2.463	24.121	-27.055	0.00	0.00	8
N	SER	B	3	1.641	24.359	-24.978	0.00	0.00	7
CA	SER	B	3	1.861	25.803	-24.995	0.00	0.00	6
CB	SER	B	3	0.530	26.545	-25.111	0.00	0.00	6
O	SER	B	3	-0.123	26.629	-23.860	0.00	0.00	8
C	SER	B	3	2.633	26.300	-23.779	0.00	0.00	6
O	SER	B	3	2.595	25.722	-22.696	0.00	0.00	8
N	SER	B	3	3.333	27.418	-23.971	0.00	0.00	7
CA	SER	B	3	4.047	28.069	-22.882	0.00	0.00	6
CB	SER	B	3	5.502	28.345	-23.261	0.00	0.00	6
O	SER	B	3	6.179	29.065	-22.245	0.00	0.00	8
C	SER	B	3	3.344	29.366	-22.501	0.00	0.00	6
O	SER	B	3	3.392	30.358	-23.233	0.00	0.00	8

**FIG. 1-43A**

O	GLU	B	3	3.007	5.069	-33.934	0.00	0.00	8
C	GLU	B	3	1.483	10.355	-32.591	0.00	0.00	6
O	GLU	B	3	0.774	10.886	-33.445	0.00	0.00	8
N	ALA	B	3	1.335	10.608	-31.294	0.00	0.00	7
CA	ALA	B	3	0.337	11.535	-30.782	0.00	0.00	6
CB	ALA	B	3	-0.199	11.071	-29.440	0.00	0.00	6
C	ALA	B	3	0.940	12.935	-30.676	0.00	0.00	6
O	ALA	B	3	0.246	13.911	-30.394	0.00	0.00	8
N	ALA	B	3	2.230	13.075	-30.953	0.00	0.00	7
CA	ALA	B	3	2.949	14.336	-30.925	0.00	0.00	6
CB	ALA	B	3	4.334	14.165	-31.539	0.00	0.00	6
C	ALA	B	3	2.209	15.465	-31.629	0.00	0.00	6
O	ALA	B	3	1.987	16.526	-31.034	0.00	0.00	8
N	SER	B	3	1.768	15.252	-32.867	0.00	0.00	7
CA	SER	B	3	1.008	16.252	-33.606	0.00	0.00	6
CB	SER	B	3	1.018	15.950	-35.105	0.00	0.00	6
O	SER	B	3	0.886	14.563	-35.359	0.00	0.00	8
C	SER	B	3	-0.427	16.377	-33.107	0.00	0.00	6
O	SER	B	3	-1.106	17.376	-33.355	0.00	0.00	8
N	ARG	B	3	-0.914	15.383	-32.386	0.00	C.10	7
CA	ARG	B	3	-2.250	15.345	-31.814	0.00	0.00	6
CB	ARG	B	3	-2.645	13.879	-31.647	0.00	0.00	6
C	ARG	B	3	-3.931	13.549	-30.920	0.00	0.00	6
C	ARG	B	3	-4.037	12.040	-30.737	0.00	0.00	6
N	THR	B	3	2.798	29.409	-21.284	0.00	0.00	7
CA	THR	B	3	2.153	30.613	-20.775	0.00	0.00	6
CB	THR	B	3	1.081	30.328	-19.712	0.00	0.00	6
O	THR	B	3	1.607	29.501	-18.667	0.00	0.00	8
C	THR	B	3	-0.111	29.623	-20.347	0.00	0.00	6
C	THR	B	3	3.171	31.612	-20.240	0.00	0.00	6
O	THR	B	3	2.842	32.728	-19.840	0.00	0.00	8
N	LYS	B	3	4.452	31.269	-20.300	0.00	0.00	7
CA	LYS	B	3	5.579	32.098	-19.939	0.00	0.00	6
CB	LYS	B	3	6.839	31.259	-19.710	0.00	0.00	6
C	LYS	B	3	6.801	30.358	-18.485	0.00	0.00	6
C	LYS	B	3	8.207	29.950	-18.071	0.00	0.00	6
CE	LYS	B	3	8.218	29.014	-16.880	0.00	0.00	6
NZ	LYS	B	3	7.415	27.785	-17.079	0.00	0.00	7
C	LYS	B	3	5.861	33.146	-21.017	0.00	0.00	6
O	LYS	B	3	6.609	34.098	-20.790	0.00	0.00	8
N	SER	B	3	5.209	33.042	-22.170	0.00	0.00	7
CA	SER	B	3	5.228	34.043	-23.217	0.00	0.00	6
CB	SER	B	3	4.676	33.493	-24.533	0.00	0.00	6
O	SER	B	3	3.444	32.822	-24.356	0.00	0.00	8
C	SER	B	3	4.449	35.293	-22.812	0.00	0.00	6
O	SER	B	3	4.735	36.385	-23.305	0.00	0.00	8
N	MET	B	3	3.481	35.155	-21.918	0.00	0.00	7
CA	MET	B	3	2.696	36.271	-21.421	0.00	0.00	6

**FIG. 1-43B**



C	HIS	B	3	11.133	31.073	-15.448	0.00	0.00	6
C	HIS	B	3	10.483	30.190	-14.655	0.00	0.00	6
N	HIS	B	3	12.426	30.601	-15.559	0.00	0.00	7
CE	HIS	B	3	12.544	29.488	-14.868	0.00	0.00	6
N	HIS	B	3	11.380	29.212	-14.307	0.00	0.00	7
C	HIS	B	3	9.253	33.231	-14.285	0.00	0.00	6
O	HIS	B	3	10.070	34.028	-13.825	0.00	0.00	8
N	LEU	B	3	8.370	32.596	-13.518	0.00	0.00	7
CA	LEU	B	3	8.182	32.913	-12.110	0.00	0.00	6
CB	LEU	B	3	6.730	32.778	-11.684	0.00	0.00	6
C	LEU	B	3	5.544	33.425	-12.363	0.00	0.00	6
C	LEU	B	3	4.547	33.915	-11.311	0.00	0.00	6
C	LEU	B	3	5.901	34.563	-13.303	0.00	0.00	6
C	LEU	B	3	9.026	32.033	-11.187	0.00	0.00	6
O	LEU	B	3	8.711	31.869	-10.007	0.00	0.00	8
N	LEU	B	3	10.095	31.456	-11.711	0.00	0.00	7
CA	LEU	B	3	11.003	30.600	-10.971	0.00	0.00	6
CB	LEU	B	3	12.016	31.480	-10.227	0.00	0.00	6
C	LEU	B	3	13.104	32.076	-11.132	0.00	0.00	6
C	LEU	B	3	13.851	33.194	-10.425	0.00	0.00	6

CB	SER	B	3	-0.321	23.253	-11.037	0.00	0.00	6
O	SER	B	3	0.888	22.520	-11.055	0.00	0.00	8
C	SER	B	3	-2.121	24.295	-12.417	0.00	0.00	6
O	SER	B	3	-3.015	23.566	-12.834	0.00	0.00	8
N	ILE	B	3	-2.337	25.530	-11.973	0.00	0.00	7
CA	ILE	B	3	-3.667	26.133	-11.972	0.00	0.00	6
CB	ILE	B	3	-3.676	27.477	-11.223	0.00	0.00	6
C	ILE	B	3	-5.031	28.162	-11.315	0.00	0.00	6
C	ILE	B	3	-3.292	27.240	-9.761	0.00	0.00	6
C	ILE	B	3	-2.987	28.470	-8.942	0.00	0.00	6
C	ILE	B	3	-4.157	26.301	-13.407	0.00	0.00	6
O	ILE	B	3	-5.243	25.828	-13.750	0.00	0.00	8
N	TYR	B	3	-3.309	26.824	-14.288	0.00	0.00	7
CA	TYR	B	3	-3.633	26.947	-15.705	0.00	0.00	6
CB	TYR	B	3	-2.493	27.567	-16.505	0.00	0.00	6
C	TYR	B	3	-1.896	28.842	-15.961	0.00	0.00	6
C	TYR	B	3	-0.581	29.179	-16.265	0.00	0.00	6
CE	TYR	B	3	-0.012	30.344	-15.788	0.00	0.00	6
C	TYR	B	3	-2.619	29.718	-15.162	0.00	0.00	6
CE	TYR	B	3	-2.057	30.876	-14.670	0.00	0.00	6

**FIG. 1-44A**







N	ARG	B	3	-13.165	27.108	-14.494	0.00	0.00	7
CZ	ARG	B	3	-13.051	28.275	-13.874	0.00	0.00	6
N	ARG	B	3	-13.379	28.396	-12.595	0.00	0.00	7
N	ARG	B	3	-12.597	29.330	-14.537	0.00	0.00	7
C	ARG	B	3	-13.421	23.828	-17.632	0.00	0.00	6
O	ARG	B	3	-14.633	23.698	-17.798	0.00	0.00	8
N	ASP	B	3	-12.690	24.638	-18.381	0.00	0.00	7
CA	ASP	B	3	-13.225	25.469	-19.440	0.00	0.00	6
CB	ASP	B	3	-12.537	26.846	-19.359	0.00	0.00	6
C	ASP	B	3	-12.948	27.685	-18.176	0.00	0.00	6
O	ASP	B	3	-13.535	27.157	-17.211	0.00	0.00	8
O	ASP	B	3	-12.682	28.908	-18.203	0.00	0.00	8
C	ASP	B	3	-12.979	24.945	-20.843	0.00	0.00	6
O	ASP	B	3	-13.300	25.620	-21.827	0.00	0.00	8
N	GLN	B	3	-12.296	23.817	-20.977	0.00	0.00	7
CA	GLN	B	3	-11.944	23.263	-22.279	0.00	0.00	6
CB	GLN	B	3	-13.126	22.512	-22.889	0.00	0.00	6
C	GLN	B	3	-13.723	21.453	-21.980	0.00	0.00	6
C	GLN	B	3	-12.920	20.174	-21.920	0.00	0.00	6
O	GLN	B	3	-12.423	19.677	-22.930	0.00	0.00	8
N	GLN	B	3	-12.779	19.616	-20.720	0.00	0.00	7

N	ASN	B	3	3.542	35.474	-29.338	0.00	0.00	7
CA	ASN	B	3	4.787	35.875	-29.954	0.00	0.00	6
CB	ASN	B	3	5.803	36.330	-28.895	0.00	0.00	6
C	ASN	B	3	5.406	37.590	-28.157	0.00	0.00	6
O	ASN	B	3	4.824	38.511	-28.729	0.00	0.00	8
N	ASN	B	3	5.713	37.619	-26.865	0.00	0.00	7
C	ASN	B	3	5.455	34.830	-30.834	0.00	0.00	6
O	ASN	B	3	6.597	35.051	-31.267	0.00	0.00	8
N	LEU	B	3	4.802	33.721	-31.152	0.00	0.00	7
CA	LEU	B	3	5.422	32.668	-31.951	0.00	0.00	6
CB	LEU	B	3	4.857	31.306	-31.559	0.00	0.00	6
C	LEU	B	3	5.462	30.051	-32.183	0.00	0.00	6
C	LEU	B	3	6.981	30.095	-32.216	0.00	0.00	6
C	LEU	B	3	4.989	28.809	-31.438	0.00	0.00	6
C	LEU	B	3	5.272	32.938	-33.443	0.00	0.00	6
O	LEU	B	3	4.492	32.311	-34.153	0.00	0.00	8
N	ASP	B	3	6.089	33.859	-33.940	0.00	0.00	7
CA	ASP	B	3	6.054	34.323	-35.311	0.00	0.00	6
CB	ASP	B	3	6.691	35.718	-35.391	0.00	0.00	6
C	ASP	B	3	5.944	36.763	-34.591	0.00	0.00	6
O	ASP	B	3	6.598	37.704	-34.092	0.00	0.00	8

**FIG. 1-45A**

C	GLN	B	3	-11.408	24.327	-23.235	0.00	0.00	6
O	GLN	B	3	-11.691	24.310	-24.433	0.00	0.00	8
N	ALA	B	3	-10.452	25.120	-22.772	0.00	0.00	7
CA	ALA	B	3	-9.774	26.140	-23.550	0.00	0.00	6
CB	ALA	B	3	-10.335	27.521	-23.267	0.00	0.00	6
C	ALA	B	3	-8.284	26.084	-23.207	0.00	0.00	6
O	ALA	B	3	-7.931	25.901	-22.041	0.00	0.00	8
N	VAL	B	3	-7.437	26.189	-24.220	0.00	0.00	7
CA	VAL	B	3	-5.993	26.123	-24.018	0.00	0.00	6
CB	VAL	B	3	-5.366	24.989	-24.847	0.00	0.00	6
C	VAL	B	3	-3.855	25.131	-24.973	0.00	0.00	6
C	VAL	B	3	-5.695	23.633	-24.230	0.00	0.00	6
C	VAL	B	3	-5.351	27.463	-24.356	0.00	0.00	6
O	VAL	B	3	-5.482	27.957	-25.472	0.00	0.00	8
N	PRO	B	3	-4.633	28.030	-23.392	0.00	0.00	7
C	PRO	B	3	-4.407	27.455	-22.044	0.00	0.00	6
CA	PRO	B	3	-3.944	29.292	-23.561	0.00	0.00	6
CB	PRO	B	3	-3.399	29.643	-22.188	0.00	0.00	6
C	PRO	B	3	-3.859	28.600	-21.245	0.00	0.00	6
C	PRO	B	3	-2.822	29.183	-24.582	0.00	0.00	6
O	PRO	B	3	-2.171	28.147	-24.703	0.00	0.00	8
N	PRO	B	3	-2.582	30.264	-25.314	0.00	0.00	7
O	ASP	B	3	4.707	36.655	-34.463	0.00	0.00	8
C	ASP	B	3	6.790	33.400	-36.271	0.00	0.00	6
O	ASP	B	3	6.462	33.348	-37.457	0.00	0.00	8
N	ASN	B	3	7.794	32.689	-35.773	0.00	0.00	7
CA	ASN	B	3	8.586	31.789	-36.597	0.00	0.00	6
CB	ASN	B	3	9.729	32.580	-37.246	0.00	0.00	6
C	ASN	B	3	9.497	32.981	-38.683	0.00	0.00	6
O	ASN	B	3	9.025	32.186	-39.498	0.00	0.00	8
N	ASN	B	3	9.828	34.229	-39.001	0.00	0.00	7
C	ASN	B	3	9.189	30.642	-35.796	0.00	0.00	6
O	ASN	B	3	10.253	30.781	-35.192	0.00	0.00	8
N	PRO	B	3	8.538	29.485	-35.827	0.00	0.00	7
C	PRO	B	3	7.263	29.247	-36.544	0.00	0.00	6
CA	PRO	B	3	9.018	28.297	-35.149	0.00	0.00	6
CB	PRO	B	3	8.089	27.190	-35.633	0.00	0.00	6
C	PRO	B	3	6.862	27.865	-36.120	0.00	0.00	6
C	PRO	B	3	10.462	27.972	-35.491	0.00	0.00	6
O	PRO	B	3	10.926	28.255	-36.597	0.00	0.00	8
N	ASP	B	3	11.178	27.374	-34.144	0.00	0.00	7
CA	ASP	B	3	12.575	26.992	-34.766	0.00	0.00	6
CB	ASP	B	3	13.194	26.503	-33.461	0.00	0.00	6
C	ASP	B	3	14.659	26.855	-33.310	0.00	0.00	6

**FIG. 1-45B**



C	CYS	B	3	8.927	21.845	-35.264	0.00	0.00	6
O	CYS	B	3	9.017	22.049	-36.482	0.00	0.00	8
N	ASP	B	3	7.998	21.058	-34.736	0.00	0.00	7
CA	ASP	B	3	6.997	20.426	-35.592	0.00	0.00	6
CB	ASP	B	3	7.556	19.082	-36.082	0.00	0.00	6
C	ASP	B	3	7.871	19.058	-37.563	0.00	0.00	6
O	ASP	B	3	8.818	19.759	-37.983	0.00	0.00	8
O	ASP	B	3	7.184	18.328	-38.308	0.00	0.00	8
C	ASP	B	3	5.677	20.184	-34.878	0.00	0.00	6
O	ASP	B	3	4.734	19.653	-35.468	0.00	0.00	8
N	LEU	B	3	5.620	20.535	-33.600	0.00	0.00	7
CA	LEU	B	3	4.427	20.303	-32.798	0.00	0.00	6
CB	LEU	B	3	4.826	20.015	-31.345	0.00	0.00	6
C	LEU	B	3	5.969	19.018	-31.137	0.00	0.00	6
C	LEU	B	3	6.737	19.332	-29.863	0.00	0.00	6
C	LEU	B	3	5.434	17.595	-31.107	0.00	0.00	6
C	LEU	B	3	3.473	21.489	-32.832	0.00	0.00	6
O	LEU	B	3	3.846	22.600	-33.214	0.00	0.00	8
N	ASP	B	3	2.236	21.241	-32.412	0.00	0.00	7
CA	ASP	B	3	1.244	22.309	-32.329	0.00	0.00	6
CB	ASP	B	3	-0.181	21.783	-32.446	0.00	0.00	6

C	GLU	B	3	-6.321	34.482	-30.651	0.00	0.00	6
C	GLU	B	3	-7.794	34.699	-30.938	0.00	0.00	6
O	GLU	B	3	-8.149	34.907	-32.118	0.00	0.00	8
O	GLU	B	3	-8.606	34.659	-29.990	0.00	0.00	8
C	GLU	B	3	-5.195	31.281	-29.152	0.00	0.00	6
O	GLU	B	3	-4.761	30.196	-29.536	0.00	0.00	8
N	ALA	B	3	-5.996	31.431	-28.105	0.00	0.00	7
CA	ALA	B	3	-6.462	30.276	-27.348	0.00	0.00	6
CB	ALA	B	3	-7.391	30.719	-26.230	0.00	0.00	6
C	ALA	B	3	-7.177	29.299	-28.276	0.00	0.00	6
O	ALA	B	3	-7.907	29.717	-29.176	0.00	0.00	8
N	ARG	B	3	-6.936	28.009	-28.069	0.00	0.00	7
CA	ARG	B	3	-7.611	26.990	-28.866	0.00	0.00	6
CB	ARG	B	3	-6.659	25.870	-29.277	0.00	0.00	6
C	ARG	B	3	-7.277	24.868	-30.241	0.00	0.00	6
C	ARG	B	3	-6.937	25.210	-31.683	0.00	0.00	6
N	ARG	B	3	-5.570	24.821	-32.015	0.00	0.00	7
CZ	ARG	B	3	-4.577	25.684	-32.190	0.00	0.00	6
N	ARG	B	3	-4.790	26.990	-32.071	0.00	0.00	7
N	ARG	B	3	-3.363	25.243	-32.490	0.00	0.00	7
C	ARG	B	3	-8.788	26.424	-28.078	0.00	0.00	6

**FIG. 1-46A**

[illegible]

**FIG. 1-46B**



O	GLU	B	3	-8.326	15.026	-17.565	0.00	0.00	8
N	TYR	B	3	-7.171	14.764	-19.474	0.00	0.00	7
CA	TYR	B	3	-5.872	14.836	-18.820	0.00	0.00	6
CB	TYR	B	3	-5.066	13.550	-19.063	0.00	0.00	6
C	TYR	B	3	-5.646	12.321	-18.401	0.00	0.00	6
C	TYR	B	3	-6.417	11.425	-19.132	0.00	0.00	6
CE	TYR	B	3	-6.978	10.312	-18.535	0.00	0.00	6
C	TYR	B	3	-5.454	12.071	-17.051	0.00	0.00	6
CE	TYR	B	3	-6.009	10.959	-16.445	0.00	0.00	6
CZ	TYR	B	3	-6.769	10.085	-17.192	0.00	0.00	6
O	TYR	B	3	-7.326	8.976	-16.597	0.00	0.00	8
C	TYR	B	3	-5.034	16.018	-19.294	0.00	0.00	6
O	TYR	B	3	-5.017	16.342	-20.482	0.00	0.00	8
N	THR	B	3	-4.282	16.626	-18.381	0.00	0.00	7
CA	THR	B	3	-3.292	17.636	-18.718	0.00	0.00	6
CB	THR	B	3	-3.692	19.082	-18.388	0.00	0.00	6
O	THR	B	3	-4.186	19.170	-17.044	0.00	0.00	8
C	THR	B	3	-4.736	19.619	-19.354	0.00	0.00	6
C	THR	B	3	-1.972	17.344	-17.995	0.00	0.00	6
O	THR	B	3	-1.947	16.819	-16.887	0.00	0.00	8
N	LEU	B	3	-0.873	17.725	-18.626	0.00	0.00	7

CA	PHE	B	4	18.387	24.746	-12.897	0.00	0.00	6
CB	PHE	B	4	18.720	26.141	-12.373	0.00	0.00	6
C	PHE	B	4	18.292	27.221	-13.330	0.00	0.00	6
C	PHE	B	4	17.267	28.087	-13.002	0.00	0.00	6
C	PHE	B	4	18.916	27.368	-14.558	0.00	0.00	6
CE	PHE	B	4	16.866	29.079	-13.876	0.00	0.00	6
CE	PHE	B	4	18.522	28.357	-15.436	0.00	0.00	6
CZ	PHE	B	4	17.495	29.215	-15.095	0.00	0.00	6
C	PHE	B	4	18.862	23.638	-11.971	0.00	0.00	6
O	PHE	B	4	18.146	23.237	-11.054	0.00	0.00	8
N	GLY	B	4	20.035	23.085	-12.261	0.00	0.00	7
CA	GLY	B	4	20.579	21.974	-11.489	0.00	0.00	6
C	GLY	B	4	20.138	20.638	-12.082	0.00	0.00	6
O	GLY	B	4	20.442	19.568	-11.554	0.00	0.00	8
N	GLY	B	4	19.372	20.671	-13.162	0.00	0.00	7
CA	GLY	B	4	18.843	19.509	-13.835	0.00	0.00	6
C	GLY	B	4	17.780	18.774	-13.036	0.00	0.00	6
O	GLY	B	4	17.658	17.555	-13.171	0.00	0.00	8
N	THR	B	4	16.986	19.478	-12.237	0.00	0.00	7
CA	THR	B	4	15.949	18.817	-11.440	0.00	0.00	6
CB	THR	B	4	15.976	19.325	-9.993	0.00	0.00	6

**FIG. 1-47A**

[illegible]

**FIG. 1-47B**





C	PHE	B	4	-3.974	18.529	-11.268	0.00	0.00	6
CE	PHE	B	4	-1.583	19.615	-12.109	0.00	0.00	6
CE	PHE	B	4	-3.142	19.154	-10.360	0.00	0.00	6
CZ	PHE	B	4	-1.948	19.701	-10.780	0.00	0.00	6
C	PHE	B	4	-5.433	15.582	-14.484	0.00	0.00	6
O	PHE	B	4	-5.299	15.351	-15.685	0.00	0.00	8
N	LYS	B	4	-6.508	15.211	-13.796	0.00	0.00	7
CA	LYS	B	4	-7.621	14.523	-14.445	0.00	0.00	6
CB	LYS	B	4	-7.615	13.048	-14.064	0.00	0.00	6
C	LYS	B	4	-8.945	12.390	-13.771	0.00	0.00	6
C	LYS	B	4	-9.066	11.022	-14.425	0.00	0.00	6
CE	LYS	B	4	-9.980	10.113	-13.620	0.00	0.00	6
NZ	LYS	B	4	-11.257	10.787	-13.251	0.00	0.00	7
C	LYS	B	4	-8.942	15.210	-14.115	0.00	0.00	6
O	LYS	B	4	-9.212	15.563	-12.970	0.00	0.00	8
N	LYS	B	4	-9.765	15.394	-15.142	0.00	0.00	7
CA	LYS	B	4	-11.067	16.029	-14.990	0.00	0.00	6
CB	LYS	B	4	-11.634	16.391	-16.366	0.00	0.00	6
C	LYS	B	4	-12.465	17.660	-16.399	0.00	0.00	6
C	LYS	B	4	-13.928	17.380	-16.089	0.00	0.00	6
CE	LYS	B	4	-14.796	18.590	-16.391	0.00	0.00	6
NZ	LYS	B	4	-14.788	19.577	-15.277	0.00	0.00	7
C	LYS	B	4	-12.043	15.106	-14.269	0.00	0.00	6
O	LYS	B	4	-12.185	13.944	-14.652	0.00	0.00	8
N	ILE	B	4	-12.698	15.610	-13.230	0.00	0.00	7
CA	ILE	B	4	-13.715	14.833	-12.522	0.00	0.00	6
CB	ILE	B	4	-13.357	14.578	-11.053	0.00	0.00	6

**FIG. 1-48A**

C	ILE	B	4	-14.584	14.417	-10.163	0.00	0.00	6
C	ILE	B	4	-12.478	13.322	-10.945	0.00	0.00	6
C	ILE	B	4	-11.906	13.091	-9.564	0.00	0.00	6
C	ILE	B	4	-15.060	15.546	-12.659	0.00	0.00	6
O	ILE	B	4	-15.481	15.769	-13.816	0.00	0.00	8
O1	WAT	W	5	4.504	27.399	-19.536	0.00	0.00	8
O1	WAT	W	5	7.437	28.629	2.535	0.00	0.00	8
O1	WAT	W	5	14.567	39.281	-19.752	0.00	0.00	8
O1	WAT	W	5	12.567	39.856	-2.839	0.00	0.00	8
O1	WAT	W	5	12.015	35.396	-4.390	0.00	0.00	8
O1	WAT	W	5	3.319	30.612	-17.061	0.00	0.00	8
O1	WAT	W	5	16.094	26.918	-5.435	0.00	0.00	8
O1	WAT	W	5	8.209	39.238	-23.056	0.00	0.00	8
O1	WAT	W	5	18.807	20.357	-7.960	0.00	0.00	8
O1	WAT	W	5	-13.395	21.538	1.565	0.00	0.00	8
O1	WAT	W	5	24.930	41.412	-15.101	0.00	0.00	8
O1	WAT	W	5	21.290	38.294	-20.198	0.00	0.00	8
O1	WAT	W	5	15.902	50.395	9.343	0.00	0.00	8

**FIG. 1-48B**

O1	WAT	W	5	-2.782	8.166	-8.701	0.00	0.00	8
O1	WAT	W	5	18.738	27.340	-19.439	0.00	0.00	8
O1	WAT	W	5	-1.747	11.046	-6.351	0.00	0.00	8
O1	WAT	W	5	6.680	14.967	-34.855	0.00	0.00	8
O1	WAT	W	5	22.057	48.723	-9.374	0.00	0.00	8
O1	WAT	W	5	-6.611	39.165	-2.117	0.00	0.00	8
O1	WAT	W	5	13.624	8.609	-12.588	0.00	0.00	8
O1	WAT	W	5	9.255	7.220	-29.727	0.00	0.00	8
O1	WAT	W	5	-5.734	12.781	-26.436	0.00	0.00	8
O1	WAT	W	5	21.680	48.304	-5.494	0.00	0.00	8
O1	WAT	W	5	15.561	45.821	-2.731	0.00	0.00	8
O1	WAT	W	5	0.642	10.760	10.232	0.00	0.00	8
O1	WAT	W	5	0.990	48.249	1.863	0.00	0.00	8
O1	WAT	W	5	20.915	17.564	-30.457	0.00	0.00	8
O1	WAT	W	5	16.863	23.110	-17.142	0.00	0.00	8
O1	WAT	W	5	9.631	43.771	-32.080	0.00	0.00	8
O1	WAT	W	5	-9.127	0.966	-13.608	0.00	0.00	8
O1	WAT	W	5	23.605	12.660	-18.246	0.00	0.00	8

**FIG. 1-48C**

N	LYS	A	2	5.691	-3.942	0.967	1.00	59.01	N
CA	LYS	A	2	6.181	-2.836	1.843	1.00	59.40	C
C	LYS	A	2	7.698	-2.690	1.729	1.00	58.26	C
O	LYS	A	2	8.433	-3.674	1.800	1.00	58.76	O
CB	LYS	A	2	5.769	-3.035	3.298	1.00	59.99	C
CG	LYS	A	2	6.542	-2.171	4.281	1.00	60.75	C
CD	LYS	A	2	5.621	-1.406	5.211	1.00	61.69	C
CE	LYS	A	2	5.333	-0.004	4.701	1.00	62.26	C
NZ	LYS	A	2	5.569	1.027	5.757	1.00	62.54	N
N	ARG	A	3	8.164	-1.457	1.572	1.00	56.23	N
CA	ARG	A	3	9.587	-1.211	1.400	1.00	54.46	C
C	ARG	A	3	10.254	-0.621	2.629	1.00	53.07	C
O	ARG	A	3	9.908	0.442	3.142	1.00	53.04	O
CB	ARG	A	3	9.797	-0.330	0.163	1.00	54.51	C
CG	ARG	A	3	9.528	-1.088	-1.137	1.00	54.53	C
CD	ARG	A	3	9.198	-0.128	-2.267	1.00	54.58	C
NE	ARG	A	3	10.369	0.430	-2.917	1.00	54.17	N
CZ	ARG	A	3	11.239	-0.232	-3.660	1.00	54.41	C
NH1	ARG	A	3	11.105	-1.535	-3.867	1.00	54.22	N
NH2	ARG	A	3	12.268	0.409	-4.208	1.00	55.03	N
N	ARG	A	4	11.255	-1.351	3.116	1.00	51.11	N
CA	ARG	A	4	12.014	-0.957	4.293	1.00	49.31	C

**FIG. 2-1A**

C	ARG	A	4		13.305	-0.261	3.888	1.00	46.70	C
O	ARG	A	4		14.075	-0.757	3.065	1.00	45.87	O
CB	ARG	A	4		12.313	-2.184	5.161	1.00	51.04	C
CG	ARG	A	4		11.082	-3.026	5.462	1.00	52.54	C
CD	ARG	A	4		11.310	-4.014	6.588	1.00	54.18	C
NE	ARG	A	4		12.714	-4.381	6.740	1.00	55.76	N
CZ	ARG	A	4		13.204	-5.089	7.754	1.00	55.81	C
NH1	ARG	A	4		12.388	-5.510	8.707	1.00	56.21	N
NH2	ARG	A	4		14.499	-5.363	7.792	1.00	56.00	N
N	VAL	A	5		13.512	0.929	4.436	1.00	44.00	N
CA	VAL	A	5		14.691	1.721	4.082	1.00	41.65	C
C	VAL	A	5		15.765	1.553	5.144	1.00	40.39	C
O	VAL	A	5		15.466	1.605	6.342	1.00	40.29	O
CB	VAL	A	5		14.334	3.204	3.904	1.00	41.18	C
CG1	VAL	A	5		15.542	4.022	3.494	1.00	40.93	C
CG2	VAL	A	5		13.215	3.337	2.878	1.00	40.99	C
N	VAL	A	6		16.989	1.323	4.687	1.00	38.36	N
CA	VAL	A	6		18.127	1.134	5.579	1.00	36.46	C

**FIG. 2-1B**

C	VAL	A	6	19.270	2.069	5.204	1.00	35.96	C
O	VAL	A	6	19.367	2.549	4.078	1.00	34.89	O
CB	VAL	A	6	18.597	-0.331	5.583	1.00	36.36	C
CG1	VAL	A	6	17.633	-1.212	6.377	1.00	35.25	C
CG2	VAL	A	6	18.774	-0.883	4.176	1.00	34.82	C
N	VAL	A	7	20.114	2.404	6.175	1.00	36.29	N
CA	VAL	A	7	21.209	3.359	5.973	1.00	34.89	C
C	VAL	A	7	22.508	2.606	5.723	1.00	35.21	C
O	VAL	A	7	23.107	2.026	6.633	1.00	34.55	O
CB	VAL	A	7	21.352	4.266	7.205	1.00	34.25	C
CG1	VAL	A	7	22.435	5.308	6.974	1.00	34.66	C
CG2	VAL	A	7	20.030	4.915	7.568	1.00	32.51	C
N	THR	A	8	22.947	2.600	4.468	1.00	35.16	N
CA	THR	A	8	24.151	1.902	4.077	1.00	34.77	C
C	THR	A	8	25.366	2.768	3.841	1.00	34.34	C
O	THR	A	8	26.312	2.285	3.191	1.00	35.61	O
CB	THR	A	8	23.893	1.120	2.751	1.00	35.46	C
OG1	THR	A	8	23.765	2.081	1.693	1.00	35.07	O
CG2	THR	A	8	22.666	0.247	2.872	1.00	34.29	C
N	GLY	A	9	25.403	4.010	4.292	1.00	33.53	N
CA	GLY	A	9	26.572	4.846	4.008	1.00	32.71	C
C	GLY	A	9	26.496	6.173	4.745	1.00	32.55	C
O	GLY	A	9	25.472	6.847	4.718	1.00	32.58	O

**FIG. 2-1C**

N	LEU	A	10	27.591	6.534	5.404	1.00	31.65	N
CA	LEU	A	10	27.691	7.753	6.182	1.00	30.79	C
C	LEU	A	10	28.815	8.653	5.700	1.00	30.11	C
O	LEU	A	10	29.837	8.168	5.209	1.00	30.41	O
CB	LEU	A	10	27.912	7.374	7.657	1.00	31.04	C
CG	LEU	A	10	26.798	6.560	8.320	1.00	31.18	C
CD1	LEU	A	10	27.208	6.161	9.736	1.00	31.32	C
CD2	LEU	A	10	25.488	7.329	8.323	1.00	30.03	C
N	GLY	A	11	28.643	9.963	5.814	1.00	29.43	N
CA	GLY	A	11	29.679	10.911	5.372	1.00	28.90	C
C	GLY	A	11	29.509	12.228	6.120	1.00	28.84	C
O	GLY	A	11	28.368	12.646	6.360	1.00	27.25	O
N	MET	A	12	30.616	12.889	6.517	1.00	29.01	N
CA	MET	A	12	30.376	14.128	7.269	1.00	29.71	C
C	MET	A	12	31.538	15.041	7.553	1.00	29.99	C
O	MET	A	12	32.635	14.675	7.959	1.00	30.94	O
CB	MET	A	12	29.709	13.689	8.579	1.00	30.44	C
CG	MET	A	12	30.111	14.370	9.851	1.00	31.28	C
SD	MET	A	12	29.114	13.787	11.236	1.00	33.04	S
CE	MET	A	12	29.030	15.291	12.208	1.00	34.14	C
N	LEU	A	13	31.255	16.339	7.480	1.00	29.20	N
CA	LEU	A	13	32.186	17.389	7.856	1.00	28.50	C

**FIG. 2-2A**



C	LEU	A	13	31.557	18.111	9.057	1.00	28.52	C
O	LEU	A	13	30.355	18.378	9.039	1.00	28.74	O
CB	LEU	A	13	32.394	18.402	6.750	1.00	28.65	C
CG	LEU	A	13	33.435	18.122	5.680	1.00	28.65	C
CD1	LEU	A	13	33.357	19.187	4.601	1.00	28.55	C
CD2	LEU	A	13	34.829	18.057	6.293	1.00	28.84	C
N	SER	A	14	32.344	18.403	10.070	1.00	28.97	N
CA	SER	A	14	31.799	19.072	11.255	1.00	28.21	C
C	SER	A	14	32.909	19.787	12.004	1.00	27.92	C
O	SER	A	14	34.097	19.551	11.780	1.00	28.19	O
CB	SER	A	14	31.141	18.044	12.170	1.00	28.44	C
OG	SER	A	14	32.052	17.670	13.191	1.00	29.39	O
N	PRO	A	15	32.515	20.647	12.923	1.00	27.64	N
CA	PRO	A	15	33.437	21.428	13.717	1.00	28.13	C
C	PRO	A	15	34.385	20.619	14.582	1.00	28.10	C
O	PRO	A	15	35.465	21.116	14.931	1.00	26.91	O
CB	PRO	A	15	32.536	22.318	14.571	1.00	28.32	C
CG	PRO	A	15	31.220	22.323	13.885	1.00	28.67	C
CD	PRO	A	15	31.096	20.981	13.207	1.00	27.90	C
N	VAL	A	16	34.019	19.402	14.975	1.00	28.38	N
CA	VAL	A	16	34.884	18.572	15.791	1.00	28.90	C

**FIG. 2-2B**

C	VAL	A	16	35.607	17.534	14.941	1.00	29.97	C
O	VAL	A	16	36.453	16.796	15.472	1.00	31.83	O
CB	VAL	A	16	34.157	17.879	16.955	1.00	28.71	C
CG1	VAL	A	16	33.534	18.907	17.896	1.00	29.04	C
CG2	VAL	A	16	33.097	16.901	16.489	1.00	28.08	C
N	GLY	A	17	35.307	17.450	13.648	1.00	29.27	N
CA	GLY	A	17	35.990	16.446	12.835	1.00	30.51	C
C	GLY	A	17	35.651	16.531	11.360	1.00	31.65	C
O	GLY	A	17	34.569	16.998	10.992	1.00	32.81	O
N	ASN	A	18	36.559	16.075	10.506	1.00	31.30	N
CA	ASN	A	18	36.365	16.100	9.062	1.00	30.77	C
C	ASN	A	18	35.892	14.767	8.528	1.00	29.51	C
O	ASN	A	18	35.733	14.560	7.319	1.00	29.78	O
CB	ASN	A	18	37.678	16.530	8.381	1.00	32.68	C
CG	ASN	A	18	37.873	18.028	8.512	1.00	35.49	C
OD1	ASN	A	18	36.915	18.750	8.815	1.00	37.19	O
ND2	ASN	A	18	39.081	18.526	8.303	1.00	36.58	N
N	THR	A	19	35.804	13.749	9.379	1.00	27.98	N
CA	THR	A	19	35.289	12.456	8.960	1.00	27.30	C
C	THR	A	19	34.258	11.975	9.989	1.00	27.68	C

**FIG. 2-2C**

O	THR	A	19	34.070	12.579	11.046	1.00	28.33	O
CB	THR	A	19	36.328	11.346	8.760	1.00	25.95	C
OG1	THR	A	19	36.898	10.987	10.030	1.00	26.38	O
CG2	THR	A	19	37.418	11.733	7.792	1.00	23.99	C
N	VAL	A	20	33.560	10.909	9.640	1.00	27.75	N
CA	VAL	A	20	32.537	10.396	10.550	1.00	28.58	C
C	VAL	A	20	33.159	9.898	11.840	1.00	30.09	C
O	VAL	A	20	32.870	10.399	12.926	1.00	31.00	O
CB	VAL	A	20	31.737	9.270	9.872	1.00	27.71	C
CG1	VAL	A	20	30.836	8.588	10.881	1.00	28.09	C
CG2	VAL	A	20	30.975	9.838	8.685	1.00	26.96	C
N	GLU	A	21	34.033	8.897	11.735	1.00	31.53	N
CA	GLU	A	21	34.669	8.328	12.915	1.00	32.01	C
C	GLU	A	21	35.385	9.347	13.770	1.00	32.56	C
O	GLU	A	21	35.216	9.306	15.005	1.00	33.46	O
CB	GLU	A	21	35.592	7.178	12.500	1.00	32.25	C
CG	GLU	A	21	34.828	6.028	11.845	1.00	32.20	C
CD	GLU	A	21	33.779	5.403	12.731	1.00	32.65	C
OE1	GLU	A	21	33.806	5.603	13.972	1.00	33.29	O

**FIG. 2-3A**

OE2	GLU	A	21	32.893	4.693	12.198	1.00	32.86	O
N	SER	A	22	36.124	10.300	13.198	1.00	32.24	N
CA	SER	A	22	36.864	11.236	14.055	1.00	31.95	C
C	SER	A	22	35.894	12.051	14.892	1.00	32.52	C
O	SER	A	22	36.024	12.198	16.107	1.00	33.65	O
CB	SER	A	22	37.774	12.135	13.245	1.00	32.45	C
OG	SER	A	22	37.164	12.619	12.073	1.00	33.99	O
N	THR	A	23	34.883	12.592	14.222	1.00	32.30	N
CA	THR	A	23	33.842	13.388	14.853	1.00	30.89	C
C	THR	A	23	33.219	12.640	16.017	1.00	30.74	C
O	THR	A	23	33.074	13.176	17.109	1.00	30.91	O
CB	THR	A	23	32.754	13.699	13.800	1.00	30.18	C
OG1	THR	A	23	33.375	14.516	12.799	1.00	30.03	O
CG2	THR	A	23	31.561	14.400	14.404	1.00	29.43	C
N	TRP	A	24	32.834	11.394	15.770	1.00	30.66	N
CA	TRP	A	24	32.248	10.519	16.775	1.00	31.12	C
C	TRP	A	24	33.139	10.322	17.989	1.00	31.58	C
O	TRP	A	24	32.633	10.269	19.117	1.00	32.40	O
CB	TRP	A	24	31.898	9.174	16.126	1.00	30.43	C
CG	TRP	A	24	31.118	8.241	16.993	1.00	29.54	C
CD1	TRP	A	24	31.407	6.936	17.273	1.00	29.43	C
CD2	TRP	A	24	29.913	8.537	17.709	1.00	29.07	C

**FIG. 2-3B**

NE1	TRP	A	24	30.455	6.403	18.106	1.00	29.04	N
CE2	TRP	A	24	29.526	7.366	18.388	1.00	28.68	C
CE3	TRP	A	24	29.120	9.680	17.823	1.00	28.43	C
CZ2	TRP	A	24	28.382	7.304	19.175	1.00	28.30	C
CZ3	TRP	A	24	27.982	9.609	18.599	1.00	28.58	C
CH2	TRP	A	24	27.623	8.433	19.274	1.00	28.30	C
N	LYS	A	25	34.456	10.210	17.816	1.00	32.36	N
CA	LYS	A	25	35.365	10.069	18.950	1.00	32.47	C
C	LYS	A	25	35.384	11.367	19.753	1.00	31.77	C
O	LYS	A	25	35.161	11.344	20.966	1.00	32.00	O
CB	LYS	A	25	36.786	9.706	18.533	1.00	34.20	C
CG	LYS	A	25	36.856	8.568	17.532	1.00	36.79	C
CD	LYS	A	25	38.162	7.795	17.623	1.00	38.74	C
CE	LYS	A	25	38.112	6.579	16.685	1.00	39.99	C
NZ	LYS	A	25	39.171	5.589	17.053	1.00	40.83	N
N	ALA	A	26	35.488	12.495	19.055	1.00	30.32	N
CA	ALA	A	26	35.467	13.791	19.718	1.00	29.97	C
C	ALA	A	26	34.201	14.001	20.527	1.00	30.40	C
O	ALA	A	26	34.274	14.526	21.654	1.00	31.66	O
CB	ALA	A	26	35.654	14.915	18.714	1.00	30.12	C
N	LEU	A	27	33.043	13.626	19.995	1.00	30.16	N
CA	LEU	A	27	31.798	13.797	20.745	1.00	30.85	C

**FIG. 2-3C**

C	LEU	A	27	31.799	12.936	22.006	1.00	31.50	C
O	LEU	A	27	31.470	13.405	23.098	1.00	31.92	O
CB	LEU	A	27	30.585	13.468	19.896	1.00	30.80	C
CG	LEU	A	27	30.244	14.307	18.673	1.00	30.36	C
CD1	LEU	A	27	28.797	14.053	18.270	1.00	30.28	C
CD2	LEU	A	27	30.456	15.790	18.910	1.00	30.98	C
N	LEU	A	28	32.181	11.666	21.869	1.00	31.46	N
CA	LEU	A	28	32.202	10.758	23.013	1.00	31.67	C
C	LEU	A	28	33.223	11.167	24.054	1.00	32.22	C
O	LEU	A	28	33.013	10.970	25.258	1.00	33.37	O
CB	LEU	A	28	32.424	9.314	22.544	1.00	30.95	C
CG	LEU	A	28	31.228	8.660	21.830	1.00	30.19	C
CD1	LEU	A	28	31.560	7.271	21.337	1.00	28.60	C
CD2	LEU	A	28	30.002	8.622	22.744	1.00	29.86	C
N	ALA	A	29	34.295	11.843	23.649	1.00	32.19	N
CA	ALA	A	29	35.302	12.346	24.565	1.00	31.97	C
C	ALA	A	29	34.965	13.745	25.063	1.00	32.74	C
O	ALA	A	29	35.830	14.417	25.632	1.00	33.76	O
CB	ALA	A	29	36.675	12.342	23.893	1.00	30.85	C

**FIG. 2-4A**

N	GLY	A	30	33.761	14.238	24.824	1.00	32.92	N
CA	GLY	A	30	33.297	15.529	25.232	1.00	33.16	C
C	GLY	A	30	34.121	16.708	24.757	1.00	34.03	C
O	GLY	A	30	34.194	17.728	25.454	1.00	33.69	O
N	GLN	A	31	34.712	16.630	23.571	1.00	35.19	N
CA	GLN	A	31	35.478	17.738	23.014	1.00	36.06	C
C	GLN	A	31	34.564	18.823	22.454	1.00	35.59	C
O	GLN	A	31	33.447	18.518	22.014	1.00	36.40	O
CB	GLN	A	31	36.414	17.217	21.915	1.00	37.41	C
CG	GLN	A	31	37.802	16.866	22.389	1.00	39.45	C
CD	GLN	A	31	38.613	16.003	21.451	1.00	40.61	C
OE1	GLN	A	31	38.690	16.219	20.241	1.00	41.07	O
NE2	GLN	A	31	39.278	14.977	21.999	1.00	41.32	N
N	SER	A	32	35.018	20.075	22.452	1.00	33.36	N
CA	SER	A	32	34.222	21.154	21.881	1.00	32.18	C
C	SER	A	32	34.851	21.584	20.549	1.00	32.02	C
O	SER	A	32	36.060	21.425	20.377	1.00	32.16	O
CB	SER	A	32	34.092	22.344	22.816	1.00	31.37	C
OG	SER	A	32	33.391	23.419	22.212	1.00	29.60	O
N	GLY	A	33	34.043	22.121	19.642	1.00	30.46	N
CA	GLY	A	33	34.570	22.558	18.354	1.00	29.56	C
C	GLY	A	33	34.467	24.072	18.211	1.00	28.85	C
O	GLY	A	33	34.791	24.628	17.163	1.00	28.54	O
N	ILE	A	34	33.969	24.719	19.253	1.00	28.51	N
CA	ILE	A	34	33.770	26.156	19.246	1.00	29.03	C

**FIG. 2-4B**

[illegible]

**FIG. 2-4C**



CD2	LEU	A	36	36.741	34.337	20.280	1.00	33.48	C
N	ILE	A	37	36.144	33.366	15.713	1.00	32.62	N
CA	ILE	A	37	36.052	33.596	14.266	1.00	32.27	C
C	ILE	A	37	37.234	34.456	13.866	1.00	33.50	C
O	ILE	A	37	37.536	35.417	14.575	1.00	34.14	O
CB	ILE	A	37	34.730	34.316	13.961	1.00	31.61	C
CG1	ILE	A	37	33.573	33.312	13.932	1.00	30.43	C
CG2	ILE	A	37	34.812	35.106	12.666	1.00	31.81	C
CD1	ILE	A	37	32.227	33.902	14.284	1.00	29.18	C
N	ASP	A	38	37.947	34.146	12.798	1.00	36.45	N
CA	ASP	A	38	39.076	35.005	12.421	1.00	38.42	C
C	ASP	A	38	39.047	35.372	10.951	1.00	38.45	C
O	ASP	A	38	39.881	36.176	10.520	1.00	38.84	O
CB	ASP	A	38	40.394	34.326	12.797	1.00	40.40	C
CG	ASP	A	38	40.402	32.903	12.257	1.00	42.60	C
OD1	ASP	A	38	40.644	32.740	11.043	1.00	43.69	O
OD2	ASP	A	38	40.106	31.982	13.045	1.00	44.53	O
N	HIS	A	39	38.003	34.975	10.218	1.00	38.59	N
CA	HIS	A	39	37.926	35.284	8.792	1.00	38.54	C
C	HIS	A	39	37.217	36.591	8.487	1.00	38.34	C
O	HIS	A	39	37.094	36.980	7.321	1.00	38.38	O

**FIG. 2-5A**

CB	HIS	A	39	37.332	34.130	7.991	1.00	38.62	C
CG	HIS	A	39	36.023	33.615	8.480	1.00	39.30	C
ND1	HIS	A	39	35.901	32.834	9.610	1.00	40.20	N
CD2	HIS	A	39	34.768	33.780	7.997	1.00	39.04	C
CE1	HIS	A	39	34.625	32.533	9.798	1.00	39.85	C
NE2	HIS	A	39	33.921	33.101	8.833	1.00	39.44	N
N	PHE	A	40	36.775	37.315	9.496	1.00	38.47	N
CA	PHE	A	40	36.168	38.633	9.305	1.00	38.57	C
C	PHE	A	40	36.307	39.420	10.609	1.00	39.55	C
O	PHE	A	40	36.427	38.804	11.671	1.00	39.71	O
CB	PHE	A	40	34.758	38.544	8.806	1.00	37.77	C
CG	PHE	A	40	33.645	38.078	9.681	1.00	36.91	C
CD1	PHE	A	40	33.136	36.796	9.553	1.00	36.30	C
CD2	PHE	A	40	33.023	38.931	10.582	1.00	36.50	C
CE1	PHE	A	40	32.078	36.365	10.325	1.00	36.32	C
CE2	PHE	A	40	31.968	38.506	11.357	1.00	36.47	C
CZ	PHE	A	40	31.493	37.215	11.240	1.00	36.21	C
N	ASP	A	41	36.441	40.735	10.523	1.00	40.59	N
CA	ASP	A	41	36.619	41.528	11.749	1.00	42.02	C
C	ASP	A	41	35.370	41.430	12.610	1.00	41.11	C
O	ASP	A	41	34.291	41.785	12.136	1.00	41.74	O
CB	ASP	A	41	36.952	42.972	11.390	1.00	43.80	C
CG	ASP	A	41	37.737	43.667	12.486	1.00	45.45	C

**FIG. 2-5B**

OD1	ASP	A	41	38.750	43.090	12.935	1.00	46.51	O
OD2	ASP	A	41	37.345	44.779	12.895	1.00	46.80	O
N	THR	A	42	35.478	40.951	13.839	1.00	40.44	N
CA	THR	A	42	34.321	40.785	14.706	1.00	40.50	C
C	THR	A	42	34.224	41.828	15.807	1.00	40.76	C
O	THR	A	42	33.347	41.734	16.675	1.00	40.62	O
CB	THR	A	42	34.295	39.379	15.352	1.00	40.02	C
OG1	THR	A	42	35.528	39.130	16.028	1.00	39.27	O
CG2	THR	A	42	34.100	38.290	14.308	1.00	39.67	C
N	SER	A	43	35.051	42.859	15.744	1.00	41.65	N
CA	SER	A	43	35.114	43.915	16.740	1.00	41.97	C
C	SER	A	43	33.764	44.533	17.050	1.00	41.66	C
O	SER	A	43	33.431	44.735	18.230	1.00	42.75	O
CB	SER	A	43	36.093	45.012	16.302	1.00	42.49	C
OG	SER	A	43	35.789	45.413	14.971	1.00	44.87	O
N	ALA	A	44	32.958	44.828	16.034	1.00	40.22	N
CA	ALA	A	44	31.642	45.406	16.288	1.00	39.07	C
C	ALA	A	44	30.582	44.357	16.589	1.00	38.38	C
O	ALA	A	44	29.423	44.734	16.810	1.00	39.11	O

**FIG. 2-5C**

CB	ALA	A	44	31.208	46.211	15.064	1.00	39.04	C
N	TYR	A	45	30.911	43.070	16.572	1.00	36.80	N
CA	TYR	A	45	29.924	42.025	16.761	1.00	35.25	C
C	TYR	A	45	29.768	41.583	18.197	1.00	34.29	C
O	TYR	A	45	30.735	41.526	18.958	1.00	35.60	O
CB	TYR	A	45	30.276	40.829	15.864	1.00	35.92	C
CG	TYR	A	45	30.039	41.091	14.391	1.00	36.02	C
CD1	TYR	A	45	30.930	41.877	13.664	1.00	36.12	C
CD2	TYR	A	45	28.944	40.551	13.727	1.00	35.78	C
CE1	TYR	A	45	30.721	42.140	12.321	1.00	35.54	C
CE2	TYR	A	45	28.735	40.799	12.380	1.00	35.49	C
CZ	TYR	A	45	29.621	41.592	11.692	1.00	35.82	C
OH	TYR	A	45	29.435	41.833	10.351	1.00	37.58	O
N	ALA	A	46	28.556	41.188	18.571	1.00	32.36	N
CA	ALA	A	46	28.245	40.750	19.929	1.00	31.00	C
C	ALA	A	46	28.587	39.287	20.162	1.00	30.09	C
O	ALA	A	46	28.536	38.763	21.281	1.00	30.77	O
CB	ALA	A	46	26.769	41.000	20.237	1.00	29.78	C
N	THR	A	47	28.832	38.560	19.098	1.00	29.39	N
CA	THR	A	47	29.274	37.171	19.162	1.00	29.14	C

**FIG. 2-6A**

C	THR	A	47	30.518	37.099	18.273	1.00	29.84	C
O	THR	A	47	30.500	37.554	17.120	1.00	29.99	O
CB	THR	A	47	28.209	36.160	18.763	1.00	28.64	C
OG1	THR	A	47	27.018	36.347	19.549	1.00	26.79	O
CG2	THR	A	47	28.730	34.739	18.992	1.00	27.92	C
N	LYS	A	48	31.607	36.614	18.844	1.00	30.40	N
CA	LYS	A	48	32.866	36.561	18.111	1.00	31.75	C
C	LYS	A	48	33.337	35.135	17.911	1.00	31.94	C
O	LYS	A	48	34.499	34.911	17.538	1.00	33.23	O
CB	LYS	A	48	33.936	37.388	18.833	1.00	33.40	C
CG	LYS	A	48	33.425	38.325	19.913	1.00	34.99	C
CD	LYS	A	48	34.435	39.384	20.296	1.00	36.14	C
CE	LYS	A	48	34.249	40.674	19.509	1.00	36.82	C
NZ	LYS	A	48	33.140	41.508	20.060	1.00	37.15	N
N	PHE	A	49	32.433	34.182	18.140	1.00	31.02	N
CA	PHE	A	49	32.807	32.777	18.010	1.00	30.48	C
C	PHE	A	49	31.747	31.913	17.344	1.00	30.81	C
O	PHE	A	49	30.561	32.225	17.292	1.00	30.88	O
CB	PHE	A	49	33.110	32.226	19.413	1.00	29.09	C
CG	PHE	A	49	31.914	32.281	20.325	1.00	28.73	C

**FIG. 2-6B**

CD1	PHE	A	49	31.032	31.225	20.409	1.00	28.37	C
CD2	PHE	A	49	31.685	33.400	21.114	1.00	28.99	C
CE1	PHE	A	49	29.947	31.281	21.267	1.00	29.19	C
CE2	PHE	A	49	30.593	33.466	21.957	1.00	28.39	C
CZ	PHE	A	49	29.720	32.401	22.041	1.00	28.17	C
N	ALA	A	50	32.193	30.761	16.845	1.00	31.01	N
CA	ALA	A	50	31.329	29.803	16.187	1.00	30.91	C
C	ALA	A	50	31.951	28.410	16.154	1.00	31.13	C
O	ALA	A	50	33.063	28.170	16.607	1.00	31.32	O
CB	ALA	A	50	31.048	30.264	14.758	1.00	30.31	C
N	GLY	A	51	31.191	27.470	15.612	1.00	31.33	N
CA	GLY	A	51	31.707	26.114	15.400	1.00	31.92	C
C	GLY	A	51	32.119	26.098	13.905	1.00	32.48	C
O	GLY	A	51	31.249	26.054	13.042	1.00	31.41	O
N	LEU	A	52	33.409	26.221	13.650	1.00	33.16	N
CA	LEU	A	52	33.924	26.250	12.289	1.00	33.73	C
C	LEU	A	52	34.613	24.952	11.886	1.00	34.33	C
O	LEU	A	52	35.176	24.241	12.710	1.00	34.72	O
CB	LEU	A	52	34.888	27.424	12.127	1.00	33.94	C
CG	LEU	A	52	34.364	28.806	12.525	1.00	34.26	C
CD1	LEU	A	52	35.497	29.657	13.078	1.00	33.88	C
CD2	LEU	A	52	33.698	29.515	11.354	1.00	33.97	C
N	VAL	A	53	34.539	24.625	10.602	1.00	35.38	N

**FIG. 2-6C**

CA	VAL	A	53	35.180	23.418	10.060	1.00	36.67	C
C	VAL	A	53	36.657	23.748	9.883	1.00	39.49	C
O	VAL	A	53	36.983	24.713	9.185	1.00	39.50	O
CB	VAL	A	53	34.492	22.991	8.765	1.00	35.64	C
CG1	VAL	A	53	35.288	21.993	7.943	1.00	34.33	C
CG2	VAL	A	53	33.113	22.403	9.098	1.00	34.62	C
N	LYS	A	54	37.535	23.040	10.588	1.00	42.77	N
CA	LYS	A	54	38.955	23.337	10.595	1.00	46.02	C
C	LYS	A	54	39.807	22.528	9.634	1.00	48.60	C
O	LYS	A	54	39.695	21.320	9.468	1.00	48.51	O
CB	LYS	A	54	39.498	23.184	12.031	1.00	46.00	C
CG	LYS	A	54	38.765	24.095	13.013	1.00	46.36	C
CD	LYS	A	54	38.735	23.509	14.408	1.00	46.28	C
CE	LYS	A	54	37.330	23.395	14.954	1.00	46.49	C
NZ	LYS	A	54	36.792	24.669	15.488	1.00	46.54	N
N	ASP	A	55	40.730	23.244	8.991	1.00	52.11	N
CA	ASP	A	55	41.654	22.694	8.012	1.00	55.06	C
C	ASP	A	55	40.927	21.790	7.030	1.00	56.01	C
O	ASP	A	55	41.110	20.579	6.985	1.00	56.42	O
CB	ASP	A	55	42.813	21.976	8.707	1.00	56.66	C
CG	ASP	A	55	43.718	22.953	9.441	1.00	58.45	C

**FIG. 2-7A**

OD1	ASP	A	55	44.364	23.795	8.777	1.00	59.28	O
OD2	ASP	A	55	43.773	22.897	10.692	1.00	59.47	O
N	PHE	A	56	40.060	22.409	6.230	1.00	57.29	N
CA	PHE	A	56	39.245	21.657	5.276	1.00	58.33	C
C	PHE	A	56	39.919	21.613	3.915	1.00	59.60	C
O	PHE	A	56	40.252	22.646	3.339	1.00	60.07	O
CB	PHE	A	56	37.845	22.257	5.201	1.00	57.68	C
CG	PHE	A	56	37.061	21.988	3.953	1.00	56.82	C
CD1	PHE	A	56	36.509	20.746	3.707	1.00	56.49	C
CD2	PHE	A	56	36.868	22.997	3.019	1.00	56.58	C
CE1	PHE	A	56	35.791	20.514	2.548	1.00	56.82	C
CE2	PHE	A	56	36.143	22.774	1.868	1.00	56.36	C
CZ	PHE	A	56	35.602	21.526	1.630	1.00	56.45	C
N	ASN	A	57	40.137	20.409	3.416	1.00	61.48	N
CA	ASN	A	57	40.716	20.206	2.094	1.00	63.34	C
C	ASN	A	57	39.632	19.660	1.162	1.00	64.04	C
O	ASN	A	57	38.720	18.963	1.625	1.00	64.29	O
CB	ASN	A	57	41.890	19.230	2.145	1.00	64.21	C
CG	ASN	A	57	43.104	19.746	1.398	1.00	65.21	C

**FIG. 2-7B**





OD1	ASP	A	60	42.745	16.618	-1.651	1.00	69.37	O
OD2	ASP	A	60	41.707	14.871	-0.819	1.00	69.27	O
N	ILE	A	61	39.022	16.292	-4.357	1.00	67.60	N
CA	ILE	A	61	37.674	16.071	-4.832	1.00	67.38	C
C	ILE	A	61	37.180	17.149	-5.787	1.00	67.54	C
O	ILE	A	61	36.497	16.848	-6.770	1.00	67.93	O
CB	ILE	A	61	36.667	15.988	-3.664	1.00	67.40	C
CG1	ILE	A	61	37.311	15.408	-2.413	1.00	67.80	C
CG2	ILE	A	61	35.449	15.180	-4.083	1.00	67.34	C
CD1	ILE	A	61	37.777	13.973	-2.513	1.00	68.03	C
N	ILE	A	62	37.391	18.412	-5.440	1.00	67.52	N
CA	ILE	A	62	36.982	19.529	-6.274	1.00	67.98	C
C	ILE	A	62	38.205	20.343	-6.706	1.00	68.48	C
O	ILE	A	62	38.999	20.776	-5.872	1.00	68.15	O
CB	ILE	A	62	35.993	20.477	-5.575	1.00	68.14	C
CG1	ILE	A	62	34.855	19.723	-4.881	1.00	67.67	C
CG2	ILE	A	62	35.412	21.476	-6.575	1.00	67.87	C
CD1	ILE	A	62	34.527	20.263	-3.510	1.00	67.28	C
N	SER	A	63	38.310	20.600	-8.002	1.00	69.51	N
CA	SER	A	63	39.417	21.370	-8.554	1.00	70.54	C
C	SER	A	63	39.290	22.856	-8.265	1.00	70.89	C
O	SER	A	63	38.176	23.377	-8.181	1.00	71.31	O
CB	SER	A	63	39.443	21.182	-10.081	1.00	71.01	C

**FIG. 2-8A**

OG	SER	A	63	38.191	21.601	-10.622	1.00	71.28	O
N	ARG	A	64	40.407	23.574	-8.237	1.00	71.13	N
CA	ARG	A	64	40.418	25.011	-7.990	1.00	70.88	C
C	ARG	A	64	39.638	25.800	-9.027	1.00	69.35	C
O	ARG	A	64	39.069	26.861	-8.737	1.00	69.23	O
CB	ARG	A	64	41.859	25.524	-7.905	1.00	72.62	C
CG	ARG	A	64	42.772	24.624	-7.080	1.00	74.72	C
CD	ARG	A	64	43.816	23.964	-7.969	1.00	76.13	C
NE	ARG	A	64	44.540	22.911	-7.262	1.00	77.32	N
CZ	ARG	A	64	45.834	22.661	-7.436	1.00	78.17	C
NH1	ARG	A	64	46.546	23.383	-8.294	1.00	78.63	N
NH2	ARG	A	64	46.395	21.679	-6.743	1.00	78.58	N
N	LYS	A	65	39.566	25.310	-10.259	1.00	67.53	N
CA	LYS	A	65	38.788	25.972	-11.298	1.00	65.69	C
C	LYS	A	65	37.295	25.760	-11.038	1.00	63.81	C
O	LYS	A	65	36.479	26.601	-11.405	1.00	63.43	O
CB	LYS	A	65	39.167	25.454	-12.682	1.00	66.44	C

**FIG. 2-8B**

CG	LYS	A	65	40.622	25.665	-13.056	1.00	67.23	C
CD	LYS	A	65	40.858	27.006	-13.722	1.00	67.48	C
CE	LYS	A	65	41.632	26.857	-15.022	1.00	67.88	C
NZ	LYS	A	65	41.367	27.998	-15.950	1.00	67.80	N
N	GLU	A	66	36.945	24.645	-10.402	1.00	61.40	N
CA	GLU	A	66	35.560	24.328	-10.097	1.00	59.42	C
C	GLU	A	66	35.121	24.864	-8.741	1.00	57.68	C
O	GLU	A	66	33.927	25.012	-8.469	1.00	57.07	O
CB	GLU	A	66	35.341	22.812	-10.174	1.00	59.70	C
CG	GLU	A	66	35.295	22.297	-11.605	1.00	60.10	C
CD	GLU	A	66	33.929	22.447	-12.245	1.00	60.14	C
OE1	GLU	A	66	33.820	23.096	-13.304	1.00	59.46	O
OE2	GLU	A	66	32.952	21.907	-11.682	1.00	60.54	O
N	GLN	A	67	36.076	25.201	-7.893	1.00	55.83	N
CA	GLN	A	67	35.842	25.754	-6.574	1.00	54.78	C
C	GLN	A	67	35.173	27.125	-6.634	1.00	53.83	C
O	GLN	A	67	34.343	27.470	-5.803	1.00	53.09	O
CB	GLN	A	67	37.175	25.908	-5.842	1.00	55.38	C
CG	GLN	A	67	37.455	24.916	-4.738	1.00	56.07	C
CD	GLN	A	67	38.776	25.233	-4.052	1.00	56.50	C
OE1	GLN	A	67	38.931	26.290	-3.447	1.00	56.45	O
NE2	GLN	A	67	39.720	24.308	-4.163	1.00	57.61	N
N	ARG	A	68	35.525	27.914	-7.632	1.00	53.40	N

**FIG. 2-8C**

CA	ARG	A	68	35.065	29.247	-7.896	1.00	52.43	C
C	ARG	A	68	33.615	29.368	-8.330	1.00	49.54	C
O	ARG	A	68	33.100	30.491	-8.400	1.00	49.30	O
CB	ARG	A	68	35.932	29.890	-9.011	1.00	55.50	C
CG	ARG	A	68	36.265	31.348	-8.741	1.00	58.96	C
CD	ARG	A	68	36.100	32.210	-9.982	1.00	61.92	C
NE	ARG	A	68	35.231	33.368	-9.770	1.00	64.11	N
CZ	ARG	A	68	35.580	34.490	-9.149	1.00	64.77	C
NH1	ARG	A	68	36.802	34.633	-8.651	1.00	65.05	N
NH2	ARG	A	68	34.710	35.487	-9.015	1.00	65.20	N
N	LYS	A	69	32.948	28.275	-8.649	1.00	45.91	N
CA	LYS	A	69	31.545	28.298	-9.044	1.00	43.05	C
C	LYS	A	69	30.648	27.848	-7.896	1.00	40.79	C
O	LYS	A	69	29.514	27.405	-8.079	1.00	40.97	O
CB	LYS	A	69	31.343	27.323	-10.216	1.00	42.96	C
CG	LYS	A	69	32.404	27.462	-11.299	1.00	43.11	C
CD	LYS	A	69	32.480	26.204	-12.151	1.00	42.58	C
CE	LYS	A	69	31.895	26.456	-13.532	1.00	42.02	C
NZ	LYS	A	69	32.812	25.970	-14.605	1.00	41.64	N
N	MET	A	70	31.191	27.869	-6.687	1.00	37.50	N
CA	MET	A	70	30.633	27.175	-5.555	1.00	34.98	C
C	MET	A	70	30.758	27.902	-4.223	1.00	32.38	C

**FIG. 2-9A**

O	MET	A	70	31.871	28.210	-3.798	1.00	32.03	O
CB	MET	A	70	31.425	25.864	-5.366	1.00	35.08	C
CG	MET	A	70	30.888	24.645	-6.066	1.00	35.01	C
SD	MET	A	70	31.957	23.217	-5.694	1.00	35.60	S
CE	MET	A	70	31.632	22.233	-7.165	1.00	35.07	C
N	ASP	A	71	29.633	28.071	-3.536	1.00	29.01	N
CA	ASP	A	71	29.750	28.647	-2.186	1.00	27.17	C
C	ASP	A	71	30.244	27.526	-1.274	1.00	26.77	C
O	ASP	A	71	30.018	26.329	-1.542	1.00	26.15	O
CB	ASP	A	71	28.432	29.242	-1.766	1.00	26.38	C
CG	ASP	A	71	28.364	29.693	-0.330	1.00	26.16	C
OD1	ASP	A	71	28.165	28.817	0.549	1.00	26.10	O
OD2	ASP	A	71	28.481	30.909	-0.081	1.00	25.93	O
N	ALA	A	72	30.909	27.882	-0.180	1.00	25.21	N
CA	ALA	A	72	31.419	26.919	0.780	1.00	23.86	C
C	ALA	A	72	30.381	25.913	1.237	1.00	23.27	C
O	ALA	A	72	30.727	24.742	1.469	1.00	23.23	O
CB	ALA	A	72	32.018	27.654	1.980	1.00	24.17	C

**FIG. 2-9B**

N	PHE	A	73	29.111	26.282	1.386	1.00	22.52	N
CA	PHE	A	73	28.109	25.289	1.788	1.00	22.41	C
C	PHE	A	73	28.012	24.159	0.777	1.00	23.21	C
O	PHE	A	73	27.924	22.992	1.186	1.00	24.39	O
CB	PHE	A	73	26.774	25.940	2.069	1.00	21.58	C
CG	PHE	A	73	25.743	25.898	0.995	1.00	20.70	C
CD1	PHE	A	73	24.736	24.944	1.023	1.00	20.86	C
CD2	PHE	A	73	25.785	26.798	-0.053	1.00	20.41	C
CE1	PHE	A	73	23.781	24.891	0.026	1.00	21.03	C
CE2	PHE	A	73	24.823	26.765	-1.046	1.00	20.99	C
CZ	PHE	A	73	23.822	25.810	-1.008	1.00	20.90	C
N	ILE	A	74	28.066	24.445	-0.515	1.00	23.43	N
CA	ILE	A	74	28.063	23.404	-1.537	1.00	24.79	C
C	ILE	A	74	29.339	22.570	-1.443	1.00	25.35	C
O	ILE	A	74	29.338	21.345	-1.565	1.00	25.40	O
CB	ILE	A	74	27.946	24.049	-2.933	1.00	25.11	C
CG1	ILE	A	74	26.533	24.620	-3.124	1.00	23.99	C
CG2	ILE	A	74	28.280	23.077	-4.053	1.00	24.54	C
CD1	ILE	A	74	26.463	25.656	-4.221	1.00	23.46	C
N	GLN	A	75	30.468	23.238	-1.217	1.00	25.23	N
CA	GLN	A	75	31.747	22.553	-1.090	1.00	26.02	C
C	GLN	A	75	31.699	21.484	-0.008	1.00	25.95	C
O	GLN	A	75	32.145	20.358	-0.216	1.00	26.78	O

**FIG. 2-9C**

CB	GLN	A	75	32.871	23.546	-0.806	1.00	26.42	C
CG	GLN	A	75	33.332	24.282	-2.062	1.00	28.06	C
CD	GLN	A	75	34.302	25.389	-1.689	1.00	29.61	C
OE1	GLN	A	75	35.078	25.201	-0.737	1.00	31.73	O
NE2	GLN	A	75	34.262	26.508	-2.390	1.00	28.55	N
N	TYR	A	76	31.183	21.843	1.155	1.00	25.75	N
CA	TYR	A	76	31.012	20.945	2.284	1.00	24.59	C
C	TYR	A	76	30.091	19.783	1.905	1.00	25.40	C
O	TYR	A	76	30.453	18.620	2.090	1.00	26.52	O
CB	TYR	A	76	30.418	21.710	3.456	1.00	23.32	C
CG	TYR	A	76	31.291	22.727	4.146	1.00	23.16	C
CD1	TYR	A	76	30.789	23.430	5.249	1.00	22.41	C
CD2	TYR	A	76	32.593	23.002	3.755	1.00	22.62	C
CE1	TYR	A	76	31.549	24.362	5.915	1.00	22.33	C
CE2	TYR	A	76	33.366	23.944	4.395	1.00	21.92	C
CZ	TYR	A	76	32.842	24.622	5.477	1.00	23.20	C
OH	TYR	A	76	33.608	25.548	6.155	1.00	22.62	O
N	GLY	A	77	28.927	20.091	1.335	1.00	24.29	N
CA	GLY	A	77	27.960	19.090	0.948	1.00	23.68	C
C	GLY	A	77	28.532	18.017	0.040	1.00	24.17	C
O	GLY	A	77	28.286	16.831	0.258	1.00	24.09	O

**FIG. 2-10A**



N	ILE	A	78	29.208	18.420	-1.031	1.00	24.69	N
CA	ILE	A	78	29.852	17.512	-1.963	1.00	24.28	C
C	ILE	A	78	30.854	16.603	-1.263	1.00	24.34	C
O	ILE	A	78	30.693	15.382	-1.276	1.00	24.29	O
CB	ILE	A	78	30.586	18.300	-3.074	1.00	24.14	C
CG1	ILE	A	78	29.568	19.116	-3.859	1.00	24.40	C
CG2	ILE	A	78	31.358	17.347	-3.975	1.00	24.03	C
CD1	ILE	A	78	30.086	19.834	-5.084	1.00	24.19	C
N	VAL	A	79	31.854	17.194	-0.603	1.00	23.70	N
CA	VAL	A	79	32.878	16.422	0.095	1.00	23.40	C
C	VAL	A	79	32.243	15.394	1.017	1.00	24.44	C
O	VAL	A	79	32.638	14.232	0.981	1.00	25.15	O
CB	VAL	A	79	33.858	17.307	0.874	1.00	23.00	C
CG1	VAL	A	79	34.656	16.524	1.907	1.00	22.25	C
CG2	VAL	A	79	34.830	18.006	-0.077	1.00	22.73	C
N	ALA	A	80	31.258	15.787	1.820	1.00	25.12	N
CA	ALA	A	80	30.575	14.849	2.700	1.00	25.90	C
C	ALA	A	80	29.765	13.840	1.895	1.00	27.36	C
O	ALA	A	80	29.609	12.695	2.314	1.00	28.42	O
CB	ALA	A	80	29.689	15.571	3.690	1.00	24.87	C
N	GLY	A	81	29.235	14.245	0.749	1.00	28.62	N

**FIG. 2-10B**

CA	GLY	A	81	28.466	13.337	-0.097	1.00	30.56	C
C	GLY	A	81	29.379	12.247	-0.652	1.00	32.31	C
O	GLY	A	81	29.048	11.061	-0.608	1.00	32.11	O
N	VAL	A	82	30.556	12.667	-1.132	1.00	32.99	N
CA	VAL	A	82	31.535	11.714	-1.646	1.00	33.88	C
C	VAL	A	82	31.827	10.661	-0.586	1.00	35.83	C
O	VAL	A	82	31.598	9.465	-0.785	1.00	37.36	O
CB	VAL	A	82	32.826	12.415	-2.082	1.00	33.65	C
CG1	VAL	A	82	33.943	11.418	-2.341	1.00	32.35	C
CG2	VAL	A	82	32.578	13.263	-3.334	1.00	33.37	C
N	GLN	A	83	32.170	11.110	0.617	1.00	36.36	N
CA	GLN	A	83	32.387	10.238	1.757	1.00	36.77	C
C	GLN	A	83	31.271	9.199	1.851	1.00	36.63	C
O	GLN	A	83	31.534	8.003	1.903	1.00	37.55	O
CB	GLN	A	83	32.437	11.041	3.056	1.00	36.97	C
CG	GLN	A	83	33.765	11.611	3.489	1.00	36.84	C
CD	GLN	A	83	33.698	12.194	4.888	1.00	38.07	C
OE1	GLN	A	83	33.123	11.581	5.796	1.00	39.74	O
NE2	GLN	A	83	34.247	13.375	5.119	1.00	37.60	N
N	ALA	A	84	30.028	9.661	1.864	1.00	36.63	N
CA	ALA	A	84	28.872	8.782	1.983	1.00	36.65	C

**FIG. 2-10C**

C	ALA	A	84	28.805	7.776	0.849	1.00	36.36	C
O	ALA	A	84	28.499	6.613	1.097	1.00	35.48	O
CB	ALA	A	84	27.592	9.595	2.089	1.00	36.13	C
N	MET	A	85	29.116	8.196	-0.367	1.00	37.76	N
CA	MET	A	85	29.111	7.287	-1.508	1.00	39.69	C
C	MET	A	85	30.223	6.257	-1.367	1.00	41.00	C
O	MET	A	85	30.009	5.060	-1.568	1.00	41.42	O
CB	MET	A	85	29.264	8.053	-2.820	1.00	40.12	C
CG	MET	A	85	28.061	8.945	-3.132	1.00	40.96	C
SD	MET	A	85	26.538	8.001	-3.315	1.00	41.36	S
CE	MET	A	85	26.973	6.931	-4.683	1.00	40.65	C
N	GLN	A	86	31.410	6.738	-0.992	1.00	42.08	N
CA	GLN	A	86	32.553	5.840	-0.817	1.00	42.74	C
C	GLN	A	86	32.252	4.822	0.259	1.00	42.97	C
O	GLN	A	86	32.169	3.616	-0.027	1.00	43.31	O
CB	GLN	A	86	33.823	6.663	-0.577	1.00	43.27	C
CG	GLN	A	86	34.312	7.257	-1.888	1.00	44.50	C
CD	GLN	A	86	35.480	8.188	-1.859	1.00	45.31	C
OE1	GLN	A	86	35.978	8.671	-0.844	1.00	45.76	O
NE2	GLN	A	86	35.975	8.516	-3.067	1.00	45.96	N
N	ASP	A	87	31.763	5.277	1.408	1.00	43.03	N
CA	ASP	A	87	31.337	4.384	2.470	1.00	44.15	C
C	ASP	A	87	30.274	3.396	2.008	1.00	45.71	C

**FIG. 2-11A**

O	ASP	A	87	30.250	2.245	2.453	1.00	46.35	O
CB	ASP	A	87	30.802	5.186	3.661	1.00	43.42	C
CG	ASP	A	87	30.677	4.330	4.904	1.00	43.34	C
OD1	ASP	A	87	31.598	3.517	5.157	1.00	44.06	O
OD2	ASP	A	87	29.677	4.458	5.632	1.00	42.70	O
N	SER	A	88	29.370	3.825	1.135	1.00	47.04	N
CA	SER	A	88	28.293	2.977	0.654	1.00	48.12	C
C	SER	A	88	28.814	1.828	-0.197	1.00	49.19	C
O	SER	A	88	28.259	0.731	-0.169	1.00	48.51	O
CB	SER	A	88	27.281	3.803	-0.145	1.00	47.96	C
OG	SER	A	88	27.686	3.947	-1.492	1.00	47.71	O
N	GLY	A	89	29.809	2.112	-1.033	1.00	50.61	N
CA	GLY	A	89	30.381	1.147	-1.945	1.00	52.39	C
C	GLY	A	89	29.514	0.870	-3.164	1.00	54.05	C
O	GLY	A	89	29.776	-0.068	-3.925	1.00	54.48	O
N	LEU	A	90	28.453	1.639	-3.374	1.00	55.16	N
CA	LEU	A	90	27.568	1.451	-4.506	1.00	56.38	C
C	LEU	A	90	28.365	1.603	-5.807	1.00	57.19	C
O	LEU	A	90	29.179	2.512	-5.927	1.00	56.97	O

**FIG. 2-11B**



N	THR	A	93	25.717	2.047	-12.489	1.00	63.87	N
CA	THR	A	93	25.781	1.551	-13.860	1.00	65.29	C
C	THR	A	93	24.654	2.175	-14.672	1.00	66.26	C
O	THR	A	93	23.741	2.769	-14.099	1.00	66.46	O
CB	THR	A	93	25.634	0.023	-13.923	1.00	65.14	C
OG1	THR	A	93	24.503	-0.374	-13.130	1.00	65.30	O
CG2	THR	A	93	26.882	-0.667	-13.413	1.00	65.19	C
N	GLU	A	94	24.678	2.020	-15.992	1.00	67.78	N
CA	GLU	A	94	23.619	2.572	-16.839	1.00	68.67	C
C	GLU	A	94	22.280	1.938	-16.473	1.00	68.05	C
O	GLU	A	94	21.220	2.554	-16.551	1.00	67.97	O
CB	GLU	A	94	23.929	2.362	-18.315	1.00	70.29	C
CG	GLU	A	94	22.964	3.053	-19.266	1.00	72.04	C
CD	GLU	A	94	23.583	4.206	-20.025	1.00	73.06	C
OE1	GLU	A	94	22.821	5.037	-20.570	1.00	73.57	O
OE2	GLU	A	94	24.827	4.302	-20.098	1.00	73.83	O
N	GLU	A	95	22.325	0.700	-15.999	1.00	67.33	N
CA	GLU	A	95	21.188	-0.051	-15.531	1.00	66.97	C
C	GLU	A	95	20.796	0.344	-14.109	1.00	64.95	C
O	GLU	A	95	19.856	-0.224	-13.548	1.00	65.38	O
CB	GLU	A	95	21.506	-1.555	-15.548	1.00	69.25	C
CG	GLU	A	95	21.836	-2.102	-16.930	1.00	71.96	C

**FIG. 2-12A**

CD	GLU	A	95	22.091	-3.597	-16.938	1.00	73.58	C
OE1	GLU	A	95	22.000	-4.233	-15.861	1.00	74.24	O
OE2	GLU	A	95	22.396	-4.174	-18.011	1.00	74.44	O
N	ASN	A	96	21.515	1.286	-13.522	1.00	61.76	N
CA	ASN	A	96	21.332	1.731	-12.162	1.00	58.00	C
C	ASN	A	96	20.938	3.195	-12.036	1.00	55.15	C
O	ASN	A	96	20.028	3.537	-11.278	1.00	54.98	O
CB	ASN	A	96	22.673	1.537	-11.409	1.00	57.96	C
CG	ASN	A	96	22.424	1.041	-10.004	1.00	58.40	C
OD1	ASN	A	96	21.416	0.373	-9.766	1.00	59.02	O
ND2	ASN	A	96	23.319	1.367	-9.087	1.00	58.61	N
N	ALA	A	97	21.635	4.072	-12.739	1.00	51.18	N
CA	ALA	A	97	21.488	5.508	-12.680	1.00	47.79	C
C	ALA	A	97	20.095	6.010	-12.346	1.00	45.31	C
O	ALA	A	97	19.902	6.772	-11.399	1.00	45.01	O
CB	ALA	A	97	21.961	6.128	-13.996	1.00	47.88	C
N	THR	A	98	19.100	5.621	-13.091	1.00	42.91	N
CA	THR	A	98	17.699	5.931	-13.000	1.00	40.62	C
C	THR	A	98	17.037	5.703	-11.661	1.00	39.36	C

**FIG. 2-12B**

[illegible]

**FIG. 2-12C**



CD1	ILE	A	100	22.465	4.568	-8.720	1.00	34.52	C
N	GLY	A	101	18.781	8.612	-6.457	1.00	34.35	N
CA	GLY	A	101	18.555	10.059	-6.465	1.00	33.77	C
C	GLY	A	101	19.240	10.769	-5.308	1.00	33.33	C
O	GLY	A	101	20.126	10.214	-4.654	1.00	33.58	O
N	ALA	A	102	18.803	11.995	-5.024	1.00	32.06	N
CA	ALA	A	102	19.383	12.798	-3.953	1.00	30.82	C
C	ALA	A	102	18.332	13.668	-3.284	1.00	29.70	C
O	ALA	A	102	17.363	14.086	-3.909	1.00	31.01	O
CB	ALA	A	102	20.516	13.678	-4.479	1.00	30.53	C
N	ALA	A	103	18.512	13.933	-1.999	1.00	28.03	N
CA	ALA	A	103	17.575	14.753	-1.230	1.00	25.22	C
C	ALA	A	103	18.363	15.540	-0.184	1.00	23.85	C
O	ALA	A	103	18.559	15.134	0.952	1.00	23.10	O
CB	ALA	A	103	16.497	13.910	-0.595	1.00	24.51	C
N	ILE	A	104	19.019	16.587	-0.671	1.00	23.05	N
CA	ILE	A	104	19.908	17.401	0.135	1.00	22.38	C
C	ILE	A	104	19.394	18.834	0.207	1.00	22.22	C
O	ILE	A	104	19.072	19.399	-0.839	1.00	22.93	O
CB	ILE	A	104	21.327	17.415	-0.478	1.00	21.90	C
CG1	ILE	A	104	21.877	15.989	-0.520	1.00	21.01	C
CG2	ILE	A	104	22.239	18.354	0.291	1.00	21.57	C

**FIG. 2-13A**

CD1	ILE	A	104	22.977	15.754	-1.509	1.00	19.64	C
N	GLY	A	105	19.352	19.406	1.402	1.00	21.16	N
CA	GLY	A	105	18.934	20.783	1.569	1.00	20.18	C
C	GLY	A	105	19.941	21.613	2.354	1.00	19.37	C
O	GLY	A	105	21.043	21.222	2.690	1.00	19.81	O
N	SER	A	106	19.528	22.815	2.693	1.00	19.13	N
CA	SER	A	106	20.275	23.799	3.448	1.00	18.03	C
C	SER	A	106	19.252	24.795	4.004	1.00	19.00	C
O	SER	A	106	18.175	24.921	3.419	1.00	19.81	O
CB	SER	A	106	21.271	24.488	2.526	1.00	17.16	C
OG	SER	A	106	22.092	25.439	3.156	1.00	15.90	O
N	GLY	A	107	19.547	25.475	5.095	1.00	19.19	N
CA	GLY	A	107	18.639	26.453	5.655	1.00	18.05	C
C	GLY	A	107	18.625	27.702	4.781	1.00	18.77	C
O	GLY	A	107	17.531	28.123	4.418	1.00	18.68	O
N	ILE	A	108	19.781	28.295	4.496	1.00	19.98	N
CA	ILE	A	108	19.854	29.517	3.697	1.00	21.92	C
C	ILE	A	108	20.795	29.409	2.502	1.00	22.33	C
O	ILE	A	108	20.837	30.295	1.645	1.00	22.50	O

**FIG. 2-13B**

CB	ILE	A	108	20.293	30.744	4.526	1.00	22.68	C
CG1	ILE	A	108	19.999	32.067	3.812	1.00	22.56	C
CG2	ILE	A	108	21.790	30.677	4.834	1.00	22.23	C
CD1	ILE	A	108	18.740	32.773	4.209	1.00	22.91	C
N	GLY	A	109	21.596	28.356	2.417	1.00	23.23	N
CA	GLY	A	109	22.490	28.191	1.282	1.00	22.77	C
C	GLY	A	109	23.618	29.206	1.299	1.00	23.95	C
O	GLY	A	109	24.325	29.369	2.302	1.00	24.99	O
N	GLY	A	110	23.968	29.728	0.119	1.00	22.53	N
CA	GLY	A	110	25.186	30.444	-0.086	1.00	21.57	C
C	GLY	A	110	25.295	31.872	0.353	1.00	21.34	C
O	GLY	A	110	25.779	32.717	-0.426	1.00	20.36	O
N	LEU	A	111	25.141	32.142	1.646	1.00	21.33	N
CA	LEU	A	111	25.285	33.486	2.183	1.00	21.06	C
C	LEU	A	111	26.612	34.144	1.839	1.00	19.97	C
O	LEU	A	111	26.655	35.343	1.573	1.00	19.87	O
CB	LEU	A	111	25.107	33.458	3.709	1.00	21.38	C
CG	LEU	A	111	23.849	34.136	4.252	1.00	21.04	C
CD1	LEU	A	111	23.966	34.302	5.758	1.00	21.27	C
CD2	LEU	A	111	23.605	35.470	3.584	1.00	20.64	C
N	GLY	A	112	27.706	33.399	1.864	1.00	19.90	N
CA	GLY	A	112	29.025	33.909	1.563	1.00	19.57	C

**FIG. 2-13C**

C	GLY	A	112	29.093	34.582	0.202	1.00	19.83	C
O	GLY	A	112	29.436	35.763	0.110	1.00	19.16	O
N	LEU	A	113	28.660	33.865	-0.835	1.00	20.37	N
CA	LEU	A	113	28.717	34.373	-2.195	1.00	21.45	C
C	LEU	A	113	27.667	35.432	-2.470	1.00	22.87	C
O	LEU	A	113	27.887	36.287	-3.349	1.00	24.10	O
CB	LEU	A	113	28.668	33.257	-3.233	1.00	21.15	C
CG	LEU	A	113	29.966	32.437	-3.379	1.00	21.11	C
CD1	LEU	A	113	29.850	31.447	-4.527	1.00	20.06	C
CD2	LEU	A	113	31.172	33.342	-3.549	1.00	20.34	C
N	ILE	A	114	26.567	35.437	-1.726	1.00	23.17	N
CA	ILE	A	114	25.566	36.481	-1.922	1.00	23.67	C
C	ILE	A	114	26.153	37.807	-1.442	1.00	24.59	C
O	ILE	A	114	26.093	38.806	-2.156	1.00	24.19	O
CB	ILE	A	114	24.246	36.209	-1.205	1.00	23.59	C
CG1	ILE	A	114	23.614	34.926	-1.749	1.00	23.20	C
CG2	ILE	A	114	23.293	37.390	-1.373	1.00	23.96	C
CD1	ILE	A	114	22.368	34.488	-1.014	1.00	22.82	C
N	GLU	A	115	26.791	37.773	-0.274	1.00	26.24	N
CA	GLU	A	115	27.382	38.995	0.283	1.00	28.37	C
C	GLU	A	115	28.485	39.536	-0.625	1.00	29.01	C
O	GLU	A	115	28.597	40.732	-0.855	1.00	28.40	O
CB	GLU	A	115	27.927	38.748	1.682	1.00	28.58	C

**FIG. 2-14A**

CG	GLU	A	115	26.918	38.301	2.723	1.00	29.16	C
CD	GLU	A	115	27.594	38.057	4.056	1.00	30.83	C
OE1	GLU	A	115	27.136	37.229	4.861	1.00	31.28	O
OE2	GLU	A	115	28.643	38.695	4.293	1.00	32.63	O
N	GLU	A	116	29.313	38.632	-1.139	1.00	30.70	N
CA	GLU	A	116	30.396	38.976	-2.041	1.00	31.25	C
C	GLU	A	116	29.865	39.618	-3.315	1.00	29.86	C
O	GLU	A	116	30.328	40.689	-3.701	1.00	29.96	O
CB	GLU	A	116	31.211	37.729	-2.396	1.00	33.77	C
CG	GLU	A	116	32.443	38.037	-3.238	1.00	37.37	C
CD	GLU	A	116	33.380	36.848	-3.326	1.00	39.87	C
OE1	GLU	A	116	33.652	36.249	-2.253	1.00	41.44	O
OE2	GLU	A	116	33.825	36.519	-4.447	1.00	40.97	O
N	ASN	A	117	28.893	38.962	-3.954	1.00	27.58	N
CA	ASN	A	117	28.342	39.520	-5.195	1.00	25.34	C
C	ASN	A	117	27.694	40.865	-4.966	1.00	25.27	C
O	ASN	A	117	28.025	41.830	-5.663	1.00	25.06	O
CB	ASN	A	117	27.401	38.518	-5.849	1.00	23.78	C

**FIG. 2-14B**

CG	ASN	A	117	28.223	37.458	-6.584	1.00	23.22	C
OD1	ASN	A	117	28.593	37.682	-7.736	1.00	23.18	O
ND2	ASN	A	117	28.516	36.354	-5.929	1.00	22.14	N
N	HIS	A	118	26.877	40.991	-3.922	1.00	25.45	N
CA	HIS	A	118	26.234	42.236	-3.569	1.00	25.44	C
C	HIS	A	118	27.235	43.361	-3.319	1.00	26.62	C
O	HIS	A	118	27.016	44.496	-3.749	1.00	26.46	O
CB	HIS	A	118	25.330	42.060	-2.335	1.00	24.14	C
CG	HIS	A	118	24.462	43.273	-2.164	1.00	23.03	C
ND1	HIS	A	118	24.589	44.116	-1.095	1.00	23.14	N
CD2	HIS	A	118	23.480	43.774	-2.955	1.00	22.09	C
CE1	HIS	A	118	23.700	45.101	-1.220	1.00	22.98	C
NE2	HIS	A	118	23.026	44.916	-2.342	1.00	22.18	N
N	THR	A	119	28.347	43.054	-2.668	1.00	27.91	N
CA	THR	A	119	29.438	43.991	-2.456	1.00	29.63	C
C	THR	A	119	29.983	44.489	-3.790	1.00	30.90	C
O	THR	A	119	29.968	45.696	-4.060	1.00	32.10	O
CB	THR	A	119	30.574	43.315	-1.665	1.00	29.98	C
OG1	THR	A	119	30.019	42.865	-0.421	1.00	30.86	O
CG2	THR	A	119	31.718	44.270	-1.392	1.00	29.85	C
N	SER	A	120	30.316	43.565	-4.687	1.00	31.36	N
CA	SER	A	120	30.777	43.912	-6.021	1.00	33.00	C

**FIG. 2-14C**

C	SER	A	120	29.769	44.800	-6.743	1.00	35.01	C
O	SER	A	120	30.150	45.758	-7.410	1.00	35.40	O
CB	SER	A	120	31.031	42.671	-6.875	1.00	32.36	C
OG	SER	A	120	32.030	41.846	-6.313	1.00	31.75	O
N	LEU	A	121	28.484	44.470	-6.627	1.00	36.66	N
CA	LEU	A	121	27.455	45.262	-7.285	1.00	38.56	C
C	LEU	A	121	27.368	46.653	-6.674	1.00	40.19	C
O	LEU	A	121	27.089	47.641	-7.348	1.00	40.35	O
CB	LEU	A	121	26.106	44.542	-7.201	1.00	37.83	C
CG	LEU	A	121	24.865	45.415	-7.442	1.00	36.97	C
CD1	LEU	A	121	24.528	45.466	-8.921	1.00	36.28	C
CD2	LEU	A	121	23.708	44.901	-6.611	1.00	36.72	C
N	MET	A	122	27.576	46.750	-5.367	1.00	43.04	N
CA	MET	A	122	27.496	48.051	-4.707	1.00	46.33	C
C	MET	A	122	28.683	48.923	-5.108	1.00	46.71	C
O	MET	A	122	28.549	50.140	-5.220	1.00	47.31	O
CB	MET	A	122	27.431	47.875	-3.198	1.00	48.07	C
CG	MET	A	122	26.196	48.466	-2.532	1.00	50.31	C
SD	MET	A	122	26.330	48.350	-0.728	1.00	53.75	S
CE	MET	A	122	26.105	50.064	-0.250	1.00	53.18	C
N	ASN	A	123	29.831	48.291	-5.337	1.00	46.45	N

**FIG. 2-15A**

CA	ASN	A	123	31.042	48.999	-5.682	1.00	46.36	C
C	ASN	A	123	31.412	49.047	-7.142	1.00	45.60	C
O	ASN	A	123	32.302	49.845	-7.489	1.00	46.39	O
CB	ASN	A	123	32.212	48.384	-4.869	1.00	47.24	C
CG	ASN	A	123	32.091	48.822	-3.415	1.00	48.06	C
OD1	ASN	A	123	32.236	48.009	-2.502	1.00	48.53	O
ND2	ASN	A	123	31.799	50.105	-3.213	1.00	48.27	N
N	GLY	A	124	30.776	48.295	-8.026	1.00	44.54	N
CA	GLY	A	124	31.149	48.300	-9.427	1.00	42.78	C
C	GLY	A	124	29.989	48.188	-10.386	1.00	42.39	C
O	GLY	A	124	30.226	48.129	-11.606	1.00	43.03	O
N	GLY	A	125	28.756	48.163	-9.898	1.00	41.26	N
CA	GLY	A	125	27.592	48.015	-10.773	1.00	40.34	C
C	GLY	A	125	27.381	46.551	-11.133	1.00	40.27	C
O	GLY	A	125	28.175	45.678	-10.790	1.00	38.53	O
N	PRO	A	126	26.332	46.262	-11.900	1.00	41.29	N
CA	PRO	A	126	25.971	44.928	-12.314	1.00	41.55	C
C	PRO	A	126	26.927	44.186	-13.211	1.00	42.21	C
O	PRO	A	126	26.762	42.964	-13.385	1.00	42.68	O

**FIG. 2-15B**



CB	PRO	A	126	24.624	45.099	-13.027	1.00	41.13	C
CG	PRO	A	126	24.577	46.524	-13.423	1.00	41.26	C
CD	PRO	A	126	25.328	47.272	-12.341	1.00	41.11	C
N	ARG	A	127	27.971	44.787	-13.754	1.00	43.43	N
CA	ARG	A	127	28.910	44.074	-14.616	1.00	44.73	C
C	ARG	A	127	29.967	43.347	-13.802	1.00	44.18	C
O	ARG	A	127	30.718	42.517	-14.326	1.00	44.09	O
CB	ARG	A	127	29.542	45.013	-15.649	1.00	46.61	C
CG	ARG	A	127	28.687	45.176	-16.901	1.00	48.61	C
CD	ARG	A	127	29.498	45.033	-18.186	1.00	50.41	C
NE	ARG	A	127	29.125	46.076	-19.138	1.00	51.94	N
CZ	ARG	A	127	29.848	47.140	-19.462	1.00	52.60	C
NH1	ARG	A	127	31.051	47.369	-18.951	1.00	52.07	N
NH2	ARG	A	127	29.335	48.004	-20.340	1.00	53.61	N
N	LYS	A	128	30.019	43.644	-12.504	1.00	43.09	N
CA	LYS	A	128	30.981	42.988	-11.625	1.00	42.41	C
C	LYS	A	128	30.360	41.793	-10.914	1.00	40.89	C
O	LYS	A	128	31.045	41.117	-10.140	1.00	41.77	O
CB	LYS	A	128	31.576	43.992	-10.640	1.00	43.33	C
CG	LYS	A	128	32.325	45.130	-11.322	1.00	44.91	C
CD	LYS	A	128	33.747	45.254	-10.788	1.00	46.28	C
CE	LYS	A	128	34.769	45.362	-11.907	1.00	46.86	C
NZ	LYS	A	128	35.099	44.039	-12.514	1.00	47.29	N

**FIG. 2-15C**

N	ILE	A	129	29.092	41.484	-11.181	1.00	38.34	N
CA	ILE	A	129	28.474	40.313	-10.586	1.00	36.66	C
C	ILE	A	129	28.951	39.043	-11.299	1.00	35.18	C
O	ILE	A	129	28.755	38.876	-12.499	1.00	35.66	O
CB	ILE	A	129	26.935	40.318	-10.646	1.00	36.26	C
CG1	ILE	A	129	26.323	41.520	-9.942	1.00	35.86	C
CG2	ILE	A	129	26.398	39.016	-10.035	1.00	35.70	C
CD1	ILE	A	129	24.803	41.547	-9.968	1.00	35.30	C
N	SER	A	130	29.478	38.080	-10.560	1.00	33.85	N
CA	SER	A	130	29.883	36.813	-11.140	1.00	31.89	C
C	SER	A	130	28.789	36.177	-11.986	1.00	32.13	C
O	SER	A	130	27.620	36.054	-11.582	1.00	33.21	O
CB	SER	A	130	30.240	35.819	-10.023	1.00	30.42	C
OG	SER	A	130	30.389	34.519	-10.587	1.00	30.47	O
N	PRO	A	131	29.191	35.552	-13.092	1.00	30.65	N
CA	PRO	A	131	28.299	34.765	-13.917	1.00	29.11	C
C	PRO	A	131	27.785	33.528	-13.200	1.00	29.02	C
O	PRO	A	131	26.776	32.955	-13.637	1.00	30.14	O
CB	PRO	A	131	29.124	34.375	-15.126	1.00	28.44	C
CG	PRO	A	131	30.409	35.087	-15.033	1.00	28.97	C
CD	PRO	A	131	30.581	35.557	-13.612	1.00	29.65	C

**FIG. 2-16A**

N	PHE	A	132	28.441	33.063	-12.136	1.00	27.36	N
CA	PHE	A	132	27.960	31.926	-11.380	1.00	27.08	C
C	PHE	A	132	27.173	32.321	-10.138	1.00	26.08	C
O	PHE	A	132	26.759	31.457	-9.349	1.00	26.45	O
CB	PHE	A	132	29.120	30.991	-10.982	1.00	27.86	C
CG	PHE	A	132	29.895	30.505	-12.182	1.00	28.13	C
CD1	PHE	A	132	31.227	30.847	-12.339	1.00	27.90	C
CD2	PHE	A	132	29.289	29.734	-13.149	1.00	27.70	C
CE1	PHE	A	132	31.920	30.424	-13.452	1.00	28.55	C
CE2	PHE	A	132	29.991	29.306	-14.261	1.00	27.80	C
CZ	PHE	A	132	31.308	29.658	-14.413	1.00	27.46	C
N	PHE	A	133	26.852	33.592	-9.954	1.00	24.74	N
CA	PHE	A	133	26.121	34.021	-8.776	1.00	24.54	C
C	PHE	A	133	24.964	33.090	-8.439	1.00	24.38	C
O	PHE	A	133	24.861	32.706	-7.272	1.00	24.96	O
CB	PHE	A	133	25.593	35.451	-8.914	1.00	24.48	C
CG	PHE	A	133	24.493	35.771	-7.943	1.00	23.58	C
CD1	PHE	A	133	24.769	35.949	-6.603	1.00	23.84	C
CD2	PHE	A	133	23.184	35.882	-8.375	1.00	23.84	C

**FIG. 2-16B**

CE1	PHE	A	133	23.751	36.246	-5.709	1.00	23.71	C
CE2	PHE	A	133	22.167	36.173	-7.492	1.00	23.70	C
CZ	PHE	A	133	22.450	36.356	-6.148	1.00	23.57	C
N	VAL	A	134	24.050	32.868	-9.381	1.00	23.61	N
CA	VAL	A	134	22.876	32.053	-9.096	1.00	22.99	C
C	VAL	A	134	23.165	30.617	-8.725	1.00	22.25	C
O	VAL	A	134	22.843	30.189	-7.616	1.00	22.24	O
CB	VAL	A	134	21.848	32.123	-10.242	1.00	22.72	C
CG1	VAL	A	134	20.659	31.215	-9.955	1.00	22.55	C
CG2	VAL	A	134	21.386	33.553	-10.432	1.00	22.11	C
N	PRO	A	135	23.800	29.826	-9.581	1.00	22.78	N
CA	PRO	A	135	24.084	28.420	-9.339	1.00	22.59	C
C	PRO	A	135	25.084	28.127	-8.241	1.00	22.00	C
O	PRO	A	135	25.281	26.982	-7.813	1.00	20.80	O
1000	CB	PRO	A	135	24.618	27.904	-10.681	1.00	22.31
1001	CG	PRO	A	135	25.145	29.121	-11.356	1.00	21.93
1002	CD	PRO	A	135	24.211	30.240	-10.954	1.00	22.09
1003	N	SER	A	136	25.773	29.170	-7.770	1.00	21.31
1004	CA	SER	A	136	26.758	29.002	-6.719	1.00	20.34
1005	C	SER	A	136	26.155	29.251	-5.348	1.00	19.91
1006	O	SER	A	136	26.823	28.970	-4.356	1.00	21.13
1007	CB	SER	A	136	27.926	29.958	-6.967	1.00	19.97
1008	OG	SER	A	136	27.646	31.272	-6.556	1.00	19.96

**FIG. 2-16C**

1009	N	THR	A	137	24.936	29.770	-5.285	1.00	18.88
1010	CA	THR	A	137	24.280	30.087	-4.040	1.00	18.15
1011	C	THR	A	137	22.985	29.351	-3.757	1.00	18.90
1012	O	THR	A	137	22.581	29.274	-2.581	1.00	18.18
1013	CB	THR	A	137	23.916	31.604	-3.999	1.00	17.20
1014	OG1	THR	A	137	23.015	31.883	-5.079	1.00	15.95
1015	CG2	THR	A	137	25.142	32.469	-4.124	1.00	17.33
1016	N	ILE	A	138	22.213	29.041	-4.804	1.00	19.45
1017	CA	ILE	A	138	20.877	28.482	-4.541	1.00	19.38
1018	C	ILE	A	138	21.020	27.139	-3.844	1.00	19.57
1019	O	ILE	A	138	21.852	26.292	-4.159	1.00	20.13
1020	CB	ILE	A	138	19.979	28.411	-5.760	1.00	19.43
1021	CG1	ILE	A	138	20.656	27.763	-6.974	1.00	20.56
1022	CG2	ILE	A	138	19.521	29.812	-6.159	1.00	20.24
1023	CD1	ILE	A	138	19.620	27.294	-7.992	1.00	21.35
1024	N	VAL	A	139	20.169	26.936	-2.869	1.00	19.63
1025	CA	VAL	A	139	20.091	25.787	-2.011	1.00	19.91
1026	C	VAL	A	139	20.157	24.438	-2.666	1.00	20.52
1027	O	VAL	A	139	20.631	23.510	-1.962	1.00	23.00
1028	CB	VAL	A	139	18.802	25.907	-1.153	1.00	19.95
1029	CG1	VAL	A	139	18.110	24.594	-0.875	1.00	20.14

**FIG. 2-17A**

1030	CG2	VAL	A	139								
1031	N	ASN	A	140	19.171	26.598	0.161	1.00	20.44			
1032	CA	ASN	A	140	19.684	24.204	-3.870	1.00	19.62			
1033	C	ASN	A	140	19.595	22.851	-4.407	1.00	20.62			
1034	O	ASN	A	140	20.832	22.390	-5.143	1.00	22.05			
1035	CB	ASN	A	140	20.998	21.205	-5.505	1.00	22.79			
1036	CG	ASN	A	140	18.333	22.766	-5.279	1.00	20.75			
1037	OD1	ASN	A	140	18.373	23.691	-6.475	1.00	21.68			
1038	ND2	ASN	A	140	18.428	24.917	-6.348	1.00	22.22			
1039	N	MET	A	141	18.366	23.136	-7.680	1.00	21.47			
1040	CA	MET	A	141	21.844	23.243	-5.265	1.00	22.68			
1041	C	MET	A	141	23.058	22.907	-6.003	1.00	22.86			
1042	O	MET	A	141	23.939	21.864	-5.363	1.00	23.14			
1043	CB	MET	A	141	24.860	21.356	-6.043	1.00	23.70			
1044	CG	MET	A	141	23.793	24.197	-6.361	1.00	23.57			
1045	SD	MET	A	141	22.939	25.084	-7.273	1.00	24.80			
1046	CE	MET	A	141	22.306	24.187	-8.701	1.00	26.52			
1047	N	VAL	A	142	23.795	23.997	-9.681	1.00	25.92			
1048	CA	VAL	A	142	23.717	21.457	-4.114	1.00	22.25			
1049	C	VAL	A	142	24.512	20.395	-3.526	1.00	22.45			
			A	142	24.079	19.083	-4.204	1.00	22.89			

**FIG. 2-17B**

1050	O	VAL	A	142	24.896	18.297	-4.674	1.00	22.97
1051	CB	VAL	A	142	24.360	20.211	-2.019	1.00	23.14
1052	CG1	VAL	A	142	25.179	19.008	-1.546	1.00	22.56
1053	CG2	VAL	A	142	24.799	21.460	-1.269	1.00	24.17
1054	N	ALA	A	143	22.756	18.911	-4.309	1.00	22.65
1055	CA	ALA	A	143	22.230	17.712	-4.972	1.00	21.73
1056	C	ALA	A	143	22.517	17.765	-6.474	1.00	21.76
1057	O	ALA	A	143	22.745	16.729	-7.096	1.00	20.55
1058	CB	ALA	A	143	20.755	17.536	-4.701	1.00	20.45
1059	N	GLY	A	144	22.521	18.971	-7.035	1.00	22.30
1060	CA	GLY	A	144	22.787	19.154	-8.455	1.00	23.35
1061	C	GLY	A	144	24.162	18.611	-8.800	1.00	25.42
1062	O	GLY	A	144	24.296	17.682	-9.596	1.00	25.76
1063	N	HIS	A	145	25.196	19.154	-8.144	1.00	26.63
1064	CA	HIS	A	145	26.554	18.700	-8.407	1.00	26.89
1065	C	HIS	A	145	26.729	17.227	-8.086	1.00	28.15
1066	O	HIS	A	145	27.448	16.535	-8.832	1.00	30.31
1067	CB	HIS	A	145	27.585	19.534	-7.650	1.00	26.46
1068	CG	HIS	A	145	27.805	20.892	-8.244	1.00	26.84
1069	ND1	HIS	A	145	27.292	22.047	-7.675	1.00	27.40
1070	CD2	HIS	A	145	28.472	21.290	-9.348	1.00	26.01
1071	CE1	HIS	A	145	27.648	23.093	-8.405	1.00	26.74

**FIG. 2-17C**

1072	NE2	HIS	A	145	28.366	22.655	-9.424	1.00	25.68
1073	N	LEU	A	146	26.131	16.715	-7.008	1.00	27.39
1074	CA	LEU	A	146	26.354	15.300	-6.698	1.00	27.60
1075	C	LEU	A	146	25.747	14.423	-7.779	1.00	27.47
1076	O	LEU	A	146	26.404	13.496	-8.264	1.00	27.20
1077	CB	LEU	A	146	25.858	14.921	-5.309	1.00	28.44
1078	CG	LEU	A	146	26.876	15.053	-4.170	1.00	28.92
1079	CD1	LEU	A	146	26.181	15.129	-2.814	1.00	28.98
1080	CD2	LEU	A	146	27.861	13.895	-4.189	1.00	28.98
1081	N	THR	A	147	24.508	14.709	-8.180	1.00	27.23
1082	CA	THR	A	147	23.882	13.907	-9.228	1.00	27.05
1083	C	THR	A	147	24.791	13.868	-10.457	1.00	28.80
1084	O	THR	A	147	25.146	12.771	-10.910	1.00	30.40
1085	CB	THR	A	147	22.496	14.423	-9.619	1.00	25.46
1086	OG1	THR	A	147	22.616	15.783	-10.043	1.00	25.22
1087	CG2	THR	A	147	21.525	14.349	-8.457	1.00	24.87
1088	N	ILE	A	148	25.193	15.019	-10.977	1.00	28.90
1089	CA	ILE	A	148	26.106	15.077	-12.110	1.00	29.46
1090	C	ILE	A	148	27.356	14.247	-11.854	1.00	30.29
1091	O	ILE	A	148	27.645	13.327	-12.620	1.00	30.71
1092	CB	ILE	A	148	26.522	16.527	-12.426	1.00	29.60
1093	CG1	ILE	A	148	25.279	17.399	-12.625	1.00	28.38

**FIG. 2-18A**



1094	CG2	ILE	A	148		27.434	16.568	-13.644	1.00	29.51
1095	CD1	ILE	A	148		25.560	18.880	-12.562	1.00	27.09
1096	N	MET	A	149		28.092	14.530	-10.789	1.00	31.24
1097	CA	MET	A	149		29.290	13.793	-10.437	1.00	32.79
1098	C	MET	A	149		29.123	12.277	-10.514	1.00	32.64
1099	O	MET	A	149		30.014	11.601	-11.042	1.00	33.82
1100	CB	MET	A	149		29.743	14.124	-9.017	1.00	35.34
1101	CG	MET	A	149		30.335	15.489	-8.763	1.00	37.46
1102	SD	MET	A	149		31.040	15.582	-7.096	1.00	39.92
1103	CE	MET	A	149		32.783	15.753	-7.480	1.00	39.57
1104	N	TYR	A	150		28.089	11.691	-9.929	1.00	31.98
1105	CA	TYR	A	150		27.938	10.243	-9.929	1.00	32.50
1106	C	TYR	A	150		26.979	9.745	-10.996	1.00	32.78
1107	O	TYR	A	150		26.625	8.561	-11.031	1.00	32.62
1108	CB	TYR	A	150		27.487	9.741	-8.543	1.00	32.88
1109	CG	TYR	A	150		28.616	9.791	-7.531	1.00	33.65
1110	CD1	TYR	A	150		28.787	10.878	-6.689	1.00	33.91
1111	CD2	TYR	A	150		29.523	8.745	-7.442	1.00	34.07

**FIG. 2-18B**

[illegible]

**FIG. 2-18C**

1135	NE	ARG	A	153	19.403	8.616	-16.922	1.00	44.39
1136	CZ	ARG	A	153	18.686	9.211	-17.887	1.00	45.81
1137	NH1	ARG	A	153	18.912	10.499	-18.149	1.00	46.89
1138	NH2	ARG	A	153	17.756	8.573	-18.571	1.00	45.33
1139	N	GLY	A	154	17.858	9.525	-10.711	1.00	30.89
1140	CA	GLY	A	154	16.596	9.388	-9.976	1.00	29.41
1141	C	GLY	A	154	16.126	10.755	-9.479	1.00	28.32
1142	O	GLY	A	154	16.662	11.805	-9.842	1.00	27.72
1143	N	PRO	A	155	15.114	10.743	-8.622	1.00	27.50
1144	CA	PRO	A	155	14.569	11.943	-8.024	1.00	27.96
1145	C	PRO	A	155	15.587	12.845	-7.363	1.00	28.74
1146	O	PRO	A	155	16.486	12.456	-6.620	1.00	28.70
1147	CB	PRO	A	155	13.558	11.412	-7.002	1.00	27.50
1148	CG	PRO	A	155	13.139	10.097	-7.577	1.00	26.81
1149	CD	PRO	A	155	14.397	9.522	-8.175	1.00	26.49
1150	N	SER	A	156	15.428	14.144	-7.570	1.00	30.55
1151	CA	SER	A	156	16.307	15.171	-7.057	1.00	31.21
1152	C	SER	A	156	15.549	16.270	-6.329	1.00	31.29
1153	O	SER	A	156	15.151	17.240	-6.995	1.00	32.20
1154	CB	SER	A	156	17.001	15.840	-8.265	1.00	32.95
1155	OG	SER	A	156	18.380	15.560	-8.281	1.00	36.38
1156	N	ILE	A	157	15.342	16.183	-5.026	1.00	30.79

**FIG. 2-19A**

1157	CA	ILE	A	157	14.683	17.270	-4.316	1.00	30.48
1158	C	ILE	A	157	15.620	17.914	-3.290	1.00	29.11
1159	O	ILE	A	157	16.697	17.404	-3.002	1.00	29.37
1160	CB	ILE	A	157	13.403	16.871	-3.567	1.00	31.29
1161	CG1	ILE	A	157	13.573	15.532	-2.850	1.00	31.57
1162	CG2	ILE	A	157	12.213	16.868	-4.511	1.00	30.63
1163	CD1	ILE	A	157	12.682	15.412	-1.625	1.00	31.50
1164	N	SER	A	158	15.176	19.043	-2.753	1.00	27.18
1165	CA	SER	A	158	15.892	19.794	-1.739	1.00	25.03
1166	C	SER	A	158	14.893	20.515	-0.823	1.00	23.56
1167	O	SER	A	158	14.220	21.451	-1.244	1.00	23.34
1168	CB	SER	A	158	16.836	20.827	-2.322	1.00	25.63
1169	OG	SER	A	158	17.772	20.304	-3.231	1.00	27.19
1170	N	ILE	A	159	14.791	20.079	0.421	1.00	22.08
1171	CA	ILE	A	159	13.877	20.732	1.364	1.00	21.08
1172	C	ILE	A	159	14.610	21.800	2.162	1.00	21.52
1173	C	ILE	A	159	15.714	21.582	2.690	1.00	22.88
1174	CB	ILE	A	159	13.225	19.698	2.295	1.00	19.94
1175	CG1	ILE	A	159	12.349	18.764	1.451	1.00	18.45

**FIG. 2-19B**

1176	CG2	ILE	A	159	12.423	20.370	3.386	1.00	19.41
1177	CDI	ILE	A	159	11.674	17.668	2.231	1.00	18.07
1178	N	ALA	A	160	14.032	22.986	2.213	1.00	20.71
1179	CA	ALA	A	160	14.620	24.115	2.917	1.00	20.75
1180	C	ALA	A	160	13.679	24.596	4.021	1.00	21.65
1181	O	ALA	A	160	12.925	25.547	3.818	1.00	21.95
1182	CB	ALA	A	160	14.891	25.245	1.943	1.00	21.36
1183	N	THR	A	161	13.742	23.921	5.166	1.00	20.97
1184	CA	THR	A	161	12.891	24.251	6.299	1.00	20.26
1185	C	THR	A	161	13.702	24.702	7.504	1.00	20.52
1186	O	THR	A	161	13.595	24.136	8.594	1.00	20.22
1187	CB	THR	A	161	12.021	23.032	6.676	1.00	19.65
1188	OG1	THR	A	161	12.783	21.838	6.532	1.00	17.83
1189	CG2	THR	A	161	10.807	22.936	5.759	1.00	19.91
1190	N	ALA	A	162	14.588	25.679	7.284	1.00	20.21
1191	CA	ALA	A	162	15.388	26.216	8.382	1.00	19.96
1192	C	ALA	A	162	16.121	25.080	9.083	1.00	21.41
1193	O	ALA	A	162	16.612	24.164	8.414	1.00	21.12
1194	CB	ALA	A	162	14.479	26.948	9.353	1.00	19.07
1195	N	CYS	A	163	16.122	25.066	10.415	1.00	21.82
1196	CA	CYS	A	163	16.785	24.038	11.185	1.00	23.27
1197	C	CYS	A	163	16.148	22.662	11.143	1.00	22.15

**FIG. 2-19C**

1198	O	CYS	A	163	16.667	21.756	11.814	1.00	21.45
1199	CB	CYS	A	163	16.880	24.441	12.673	1.00	24.71
1200	SG	CYS	A	163	17.913	25.911	12.915	1.00	28.93
1201	N	THR	A	164	15.037	22.488	10.446	1.00	21.76
1202	CA	THR	A	164	14.453	21.156	10.329	1.00	21.16
1203	C	THR	A	164	14.888	20.517	9.020	1.00	20.59
1204	O	THR	A	164	14.714	19.323	8.840	1.00	20.83
1205	CB	THR	A	164	12.927	21.172	10.433	1.00	20.78
1206	OG1	THR	A	164	12.549	22.030	11.519	1.00	21.06
1207	CG2	THR	A	164	12.396	19.772	10.675	1.00	20.38
1208	N	SER	A	165	15.513	21.302	8.153	1.00	21.25
1209	CA	SER	A	165	15.984	20.830	6.858	1.00	21.35
1210	C	SER	A	165	16.609	19.451	6.925	1.00	21.57
1211	O	SER	A	165	16.155	18.544	6.235	1.00	21.53
1212	CB	SER	A	165	17.007	21.809	6.265	1.00	20.98
1213	OG	SER	A	165	16.371	23.066	6.071	1.00	21.82
1214	N	GLY	A	166	17.618	19.286	7.774	1.00	22.48
1215	CA	GLY	A	166	18.315	18.020	7.925	1.00	22.79
1216	C	GLY	A	166	17.388	16.830	8.069	1.00	22.94
1217	O	GLY	A	166	17.567	15.809	7.409	1.00	22.55
1218	N	VAL	A	167	16.444	16.936	9.004	1.00	23.72
1219	CA	VAL	A	167	15.506	15.848	9.271	1.00	24.29
1220	C	VAL	A	167	14.558	15.638	8.109	1.00	24.54
1221	O	VAL	A	167	14.389	14.509	7.627	1.00	26.12

**FIG. 2-20A**

1222	CB	VAL	A	167	14.767	16.094	10.592	1.00	24.57
1223	CG1	VAL	A	167	13.442	15.358	10.672	1.00	25.23
1224	CG2	VAL	A	167	15.675	15.663	11.743	1.00	24.67
1225	N	HIS	A	168	13.991	16.711	7.572	1.00	24.23
1226	CA	HIS	A	168	13.060	16.594	6.455	1.00	23.72
1227	C	HIS	A	168	13.671	15.915	5.243	1.00	23.37
1228	O	HIS	A	168	13.003	15.055	4.637	1.00	24.37
1229	CB	HIS	A	168	12.494	17.964	6.099	1.00	23.34
1230	CG	HIS	A	168	11.429	18.457	7.027	1.00	23.31
1231	ND1	HIS	A	168	11.102	19.797	7.120	1.00	22.78
1232	CD2	HIS	A	168	10.613	17.813	7.897	1.00	22.79
1233	CE1	HIS	A	168	10.138	19.951	8.014	1.00	22.01
1234	NE2	HIS	A	168	9.823	18.768	8.491	1.00	21.89
1235	N	ASN	A	169	14.898	16.225	4.857	1.00	22.74
1236	CA	ASN	A	169	15.502	15.616	3.663	1.00	23.00
1237	C	ASN	A	169	15.656	14.107	3.822	1.00	23.66
1238	O	ASN	A	169	15.361	13.299	2.934	1.00	23.83
1239	CB	ASN	A	169	16.826	16.291	3.343	1.00	22.66

**FIG. 2-20B**





1261	ND1	HIS	A	172	9.944	15.054	3.631	1.00	23.32
1262	CD2	HIS	A	172	8.513	14.044	2.327	1.00	22.72
1263	CE1	HIS	A	172	8.734	15.323	4.101	1.00	23.47
1264	NE2	HIS	A	172	7.844	14.717	3.329	1.00	23.29
1265	N	ALA	A	173	13.468	11.384	1.760	1.00	23.72
1266	CA	ALA	A	173	14.295	10.496	0.929	1.00	23.93
1267	C	ALA	A	173	13.810	9.058	1.148	1.00	23.83
1268	O	ALA	A	173	13.592	8.348	0.172	1.00	22.86
1269	CB	ALA	A	173	15.756	10.702	1.222	1.00	23.75
1270	N	ALA	A	174	13.506	8.691	2.390	1.00	23.88
1271	CA	ALA	A	174	12.985	7.375	2.714	1.00	24.96
1272	C	ALA	A	174	11.596	7.165	2.100	1.00	26.35
1273	O	ALA	A	174	11.326	6.134	1.482	1.00	26.24
1274	CB	ALA	A	174	12.865	7.184	4.215	1.00	24.24
1275	N	ARG	A	175	10.748	8.179	2.291	1.00	26.16
1276	CA	ARG	A	175	9.394	8.145	1.742	1.00	25.10
1277	C	ARG	A	175	9.481	7.878	0.245	1.00	27.12
1278	O	ARG	A	175	9.021	6.838	-0.251	1.00	28.18
1279	CB	ARG	A	175	8.673	9.443	2.042	1.00	23.30
1280	CG	ARG	A	175	8.348	9.684	3.507	1.00	23.23
1281	CD	ARG	A	175	7.206	8.809	3.977	1.00	23.38

**FIG. 2-21A**

1282	NE	ARG	A	175	6.465	9.357	5.099	1.00	24.63
1283	CZ	ARG	A	175	6.601	8.994	6.376	1.00	24.68
1284	NH1	ARG	A	175	7.476	8.054	6.731	1.00	24.38
1285	NH2	ARG	A	175	5.855	9.564	7.315	1.00	23.89
1286	N	ILE	A	176	10.257	8.703	-0.472	1.00	27.46
1287	CA	ILE	A	176	10.475	8.452	-1.893	1.00	27.19
1288	C	ILE	A	176	10.815	6.991	-2.141	1.00	28.06
1289	O	ILE	A	176	10.169	6.352	-2.971	1.00	29.01
1290	CB	ILE	A	176	11.568	9.372	-2.460	1.00	26.47
1291	CG1	ILE	A	176	11.036	10.812	-2.486	1.00	26.78
1292	CG2	ILE	A	176	12.020	8.935	-3.838	1.00	24.93
1293	CD1	ILE	A	176	11.966	11.826	-3.111	1.00	26.82
1294	N	ILE	A	177	11.823	6.460	-1.463	1.00	28.98
1295	CA	ILE	A	177	12.249	5.076	-1.652	1.00	29.01
1296	C	ILE	A	177	11.104	4.111	-1.387	1.00	29.49
1297	O	ILE	A	177	10.698	3.373	-2.290	1.00	30.21
1298	CB	ILE	A	177	13.483	4.745	-0.802	1.00	28.06
1299	CG1	ILE	A	177	14.718	5.428	-1.400	1.00	27.28
1300	CG2	ILE	A	177	13.712	3.245	-0.714	1.00	28.49

**FIG. 2-21B**

1301	CD1	ILE	A	177	15.924	5.483	-0.490	1.00	26.54
1302	N	ALA	A	178	10.479	4.215	-0.232	1.00	29.79
1303	CA	ALA	A	178	9.318	3.437	0.141	1.00	30.54
1304	C	ALA	A	178	8.251	3.453	-0.942	1.00	33.08
1305	O	ALA	A	178	7.640	2.422	-1.259	1.00	35.55
1306	CB	ALA	A	178	8.744	3.986	1.448	1.00	28.37
1307	N	TYR	A	179	7.975	4.621	-1.514	1.00	33.83
1308	CA	TYR	A	179	6.967	4.771	-2.546	1.00	33.95
1309	C	TYR	A	179	7.321	3.984	-3.798	1.00	33.95
1310	O	TYR	A	179	6.399	3.530	-4.495	1.00	35.65
1311	CB	TYR	A	179	6.779	6.254	-2.886	1.00	34.35
1312	CG	TYR	A	179	5.600	6.559	-3.781	1.00	34.82
1313	CD1	TYR	A	179	4.368	6.895	-3.228	1.00	35.00
1314	CD2	TYR	A	179	5.715	6.518	-5.167	1.00	34.57
1315	CE1	TYR	A	179	3.283	7.174	-4.034	1.00	35.41
1316	CE2	TYR	A	179	4.636	6.794	-5.976	1.00	34.96
1317	CZ	TYR	A	179	3.423	7.119	-5.404	1.00	35.48
1318	OH	TYR	A	179	2.338	7.399	-6.205	1.00	36.21
1319	N	GLY	A	180	8.590	3.866	-4.149	1.00	33.30
1320	CA	GLY	A	180	8.991	3.165	-5.356	1.00	33.89
1321	C	GLY	A	180	9.629	4.044	-6.418	1.00	34.58
1322	O	GLY	A	180	10.091	3.541	-7.461	1.00	34.05
1323	N	ASP	A	181	9.796	5.342	-6.136	1.00	34.25

**FIG. 2-21C**

1324	CA	ASP	A	181	10.383	6.259	-7.105	1.00	34.14
1325	C	ASP	A	181	11.898	6.108	-7.189	1.00	34.08
1326	O	ASP	A	181	12.531	6.521	-8.164	1.00	32.76
1327	CB	ASP	A	181	10.023	7.712	-6.773	1.00	34.55
1328	CG	ASP	A	181	8.564	8.032	-7.022	1.00	35.35
1329	OD1	ASP	A	181	7.996	8.921	-6.347	1.00	35.15
1330	OD2	ASP	A	181	7.975	7.377	-7.915	1.00	36.69
1331	N	ALA	A	182	12.486	5.534	-6.145	1.00	34.99
1332	CA	ALA	A	182	13.926	5.339	-6.075	1.00	35.64
1333	C	ALA	A	182	14.284	4.134	-5.210	1.00	36.12
1334	O	ALA	A	182	13.482	3.675	-4.395	1.00	36.49
1335	CB	ALA	A	182	14.594	6.592	-5.527	1.00	34.86
1336	N	ASP	A	183	15.496	3.630	-5.413	1.00	37.16
1337	CA	ASP	A	183	15.993	2.489	-4.644	1.00	37.73
1338	C	ASP	A	183	17.068	2.946	-3.662	1.00	37.03
1339	O	ASP	A	183	17.237	2.401	-2.575	1.00	37.13
1340	CB	ASP	A	183	16.558	1.416	-5.579	1.00	38.47
1341	CG	ASP	A	183	15.452	0.660	-6.299	1.00	39.28
1342	OD1	ASP	A	183	15.650	0.298	-7.477	1.00	39.31
1343	OD2	ASP	A	183	14.382	0.452	-5.672	1.00	39.27
1344	N	VAL	A	184	17.870	3.907	-4.112	1.00	35.93
1345	CA	VAL	A	184	18.906	4.529	-3.313	1.00	34.94

**FIG. 2-22A**

1346	C	VAL	A	184		18.726	6.051	-3.354	1.00	34.49
1347	O	VAL	A	184		18.388	6.611	-4.397	1.00	34.37
1348	CB	VAL	A	184		20.329	4.191	-3.783	1.00	34.92
1349	CG1	VAL	A	184		21.361	4.899	-2.904	1.00	34.98
1350	CG2	VAL	A	184		20.598	2.699	-3.774	1.00	34.24
1351	N	MET	A	185		18.909	6.700	-2.208	1.00	33.85
1352	CA	MET	A	185		18.808	8.150	-2.102	1.00	32.05
1353	C	MET	A	185		19.974	8.691	-1.280	1.00	30.49
1354	O	MET	A	185		20.234	8.138	-0.210	1.00	31.31
1355	CB	MET	A	185		17.503	8.560	-1.421	1.00	32.72
1356	CG	MET	A	185		16.248	8.454	-2.273	1.00	32.82
1357	SD	MET	A	185		16.312	9.494	-3.751	1.00	32.53
1358	CE	MET	A	185		15.762	11.052	-3.035	1.00	33.06
1359	N	VAL	A	186		20.675	9.701	-1.759	1.00	29.07
1360	CA	VAL	A	186		21.696	10.370	-0.952	1.00	27.75
1361	C	VAL	A	186		20.996	11.510	-0.206	1.00	26.95
1362	O	VAL	A	186		20.426	12.381	-0.880	1.00	28.24
1363	CB	VAL	A	186		22.846	10.975	-1.755	1.00	27.97
1364	CG1	VAL	A	186		24.006	11.307	-0.815	1.00	27.63

**FIG. 2-22B**

1365	CG2	VAL	A	186	23.324	10.065	-2.869	1.00	28.61
1366	N	ALA	A	187	20.997	11.526	1.114	1.00	24.74
1367	CA	ALA	A	187	20.259	12.588	1.793	1.00	24.07
1368	C	ALA	A	187	21.001	13.252	2.926	1.00	24.02
1369	O	ALA	A	187	21.836	12.664	3.607	1.00	24.74
1370	CB	ALA	A	187	18.942	12.013	2.304	1.00	23.14
1371	N	GLY	A	188	20.682	14.533	3.152	1.00	23.56
1372	CA	GLY	A	188	21.322	15.219	4.282	1.00	22.93
1373	C	GLY	A	188	21.198	16.719	4.107	1.00	21.97
1374	O	GLY	A	188	20.352	17.169	3.340	1.00	21.88
1375	N	GLY	A	189	22.084	17.456	4.773	1.00	21.27
1376	CA	GLY	A	189	22.026	18.915	4.623	1.00	20.91
1377	C	GLY	A	189	23.423	19.489	4.781	1.00	20.13
1378	O	GLY	A	189	24.305	18.799	5.280	1.00	20.88
1379	N	ALA	A	190	23.609	20.703	4.295	1.00	19.89
1380	CA	ALA	A	190	24.906	21.374	4.431	1.00	19.71
1381	C	ALA	A	190	24.625	22.835	4.771	1.00	19.51
1382	O	ALA	A	190	23.617	23.366	4.289	1.00	19.85
1383	CB	ALA	A	190	25.739	21.242	3.172	1.00	19.10
1384	N	GLU	A	191	25.446	23.431	5.617	1.00	19.12
1385	CA	GLU	A	191	25.249	24.825	5.981	1.00	19.12
1386	C	GLU	A	191	26.585	25.504	6.260	1.00	18.78

**FIG. 2-22C**

1387	O	GLU	A	191	27.522	24.903	6.772	1.00	18.20
1388	CB	GLU	A	191	24.313	24.973	7.186	1.00	18.97
1389	CG	GLU	A	191	23.760	26.391	7.329	1.00	20.04
1390	CD	GLU	A	191	22.420	26.607	6.662	1.00	20.10
1391	OE1	GLU	A	191	22.312	27.479	5.775	1.00	20.35
1392	OE2	GLU	A	191	21.423	25.921	6.984	1.00	19.18
1393	N	LYS	A	192	26.650	26.784	5.942	1.00	18.47
1394	CA	LYS	A	192	27.831	27.586	6.205	1.00	18.91
1395	C	LYS	A	192	27.392	29.047	6.334	1.00	19.50
1396	O	LYS	A	192	27.558	29.853	5.424	1.00	18.72
1397	CB	LYS	A	192	28.882	27.398	5.129	1.00	20.21
1398	CG	LYS	A	192	30.311	27.620	5.611	1.00	21.28
1399	CD	LYS	A	192	30.626	29.114	5.727	1.00	20.99
1400	CE	LYS	A	192	32.101	29.304	6.035	1.00	21.43
1401	NZ	LYS	A	192	32.369	30.319	7.082	1.00	20.87
1402	N	ALA	A	193	26.769	29.332	7.486	1.00	19.33
1403	CA	ALA	A	193	26.218	30.651	7.745	1.00	18.76
1404	C	ALA	A	193	27.125	31.471	8.633	1.00	20.38
1405	O	ALA	A	193	26.765	32.618	8.971	1.00	22.59
1406	CB	ALA	A	193	24.820	30.556	8.351	1.00	16.60
1407	N	SER	A	194	28.319	31.002	8.993	1.00	20.01
1408	CA	SER	A	194	29.212	31.816	9.822	1.00	19.73

**FIG. 2-23A**

1409	C	SER	A	194	29.827	32.946	9.010	1.00	19.70
1410	O	SER	A	194	31.018	32.969	8.692	1.00	19.94
1411	CB	SER	A	194	30.324	30.953	10.417	1.00	20.42
1412	OG	SER	A	194	31.139	30.457	9.359	1.00	20.95
1413	N	THR	A	195	29.005	33.897	8.600	1.00	19.16
1414	CA	THR	A	195	29.367	35.036	7.795	1.00	19.39
1415	C	THR	A	195	28.812	36.284	8.470	1.00	19.65
1416	O	THR	A	195	27.838	36.181	9.227	1.00	21.37
1417	CB	THR	A	195	28.757	34.967	6.382	1.00	20.32
1418	OG1	THR	A	195	27.366	35.354	6.457	1.00	21.29
1419	CG2	THR	A	195	28.843	33.585	5.772	1.00	19.40
1420	N	PRO	A	196	29.327	37.442	8.125	1.00	19.54
1421	CA	PRO	A	196	28.846	38.693	8.699	1.00	19.97
1422	C	PRO	A	196	27.341	38.754	8.825	1.00	19.83
1423	O	PRO	A	196	26.816	38.911	9.924	1.00	20.28
1424	CB	PRO	A	196	29.417	39.747	7.753	1.00	19.47
1425	CG	PRO	A	196	30.666	39.142	7.224	1.00	17.90
1426	CD	PRO	A	196	30.447	37.658	7.185	1.00	18.39

**FIG. 2-23B**



[illegible]

**FIG. 2-23C**

1450	N	GLY	A	201	22.885	38.974	11.615	1.00	25.48
1451	CA	GLY	A	201	21.478	38.693	11.546	1.00	25.31
1452	C	GLY	A	201	20.889	37.981	12.738	1.00	25.85
1453	O	GLY	A	201	19.849	38.418	13.259	1.00	25.85
1454	N	PHE	A	202	21.504	36.891	13.204	1.00	25.57
1455	CA	PHE	A	202	20.975	36.198	14.378	1.00	26.27
1456	C	PHE	A	202	21.237	37.041	15.627	1.00	27.19
1457	O	PHE	A	202	20.509	36.959	16.608	1.00	28.35
1458	CB	PHE	A	202	21.580	34.811	14.551	1.00	26.19
1459	CG	PHE	A	202	20.943	33.711	13.752	1.00	25.12
1460	CD1	PHE	A	202	21.643	33.073	12.738	1.00	24.21
1461	CD2	PHE	A	202	19.632	33.332	13.996	1.00	24.42
1462	CE1	PHE	A	202	21.051	32.076	11.991	1.00	23.44
1463	CE2	PHE	A	202	19.038	32.320	13.267	1.00	24.39
1464	CZ	PHE	A	202	19.752	31.695	12.257	1.00	23.79
1465	N	GLY	A	203	22.305	37.834	15.611	1.00	28.07
1466	CA	GLY	A	203	22.617	38.752	16.703	1.00	28.36
1467	C	GLY	A	203	21.489	39.776	16.825	1.00	29.38
1468	O	GLY	A	203	20.966	40.052	17.911	1.00	30.32
1469	N	ALA	A	204	21.089	40.312	15.677	1.00	28.66
1470	CA	ALA	A	204	20.027	41.289	15.581	1.00	28.43
1471	C	ALA	A	204	18.768	40.815	16.294	1.00	28.66

**FIG. 2-24A**

1472	O	ALA	A		204		18.131	41.610	16.982	1.00	29.26
1473	CB	ALA	A		204		19.743	41.609	14.117	1.00	28.52
1474	N	ALA	A		205		18.435	39.539	16.198	1.00	29.22
1475	CA	ALA	A		205		17.292	38.917	16.821	1.00	29.54
1476	C	ALA	A		205		17.532	38.582	18.293	1.00	30.76
1477	O	ALA	A		205		16.604	38.153	18.987	1.00	31.16
1478	CB	ALA	A		205		16.930	37.619	16.106	1.00	28.27
1479	N	ARG	A		206		18.779	38.677	18.735	1.00	31.45
1480	CA	ARG	A		206		19.159	38.399	20.110	1.00	32.71
1481	C	ARG	A		206		19.060	36.919	20.439	1.00	32.08
1482	O	ARG	A		206		18.810	36.532	21.575	1.00	32.74
1483	CB	ARG	A		206		18.299	39.212	21.090	1.00	33.69
1484	CG	ARG	A		206		18.709	40.680	21.147	1.00	35.43
1485	CD	ARG	A		206		18.168	41.326	22.416	1.00	37.32
1486	NE	ARG	A		206		18.714	40.674	23.601	1.00	38.75
1487	CZ	ARG	A		206		18.015	40.193	24.619	1.00	39.28
1488	NH1	ARG	A		206		18.676	39.617	25.623	1.00	40.09
1489	NH2	ARG	A		206		16.692	40.273	24.653	1.00	39.00

**FIG. 2-24B**

1490	N	ALA	A	207		19.351	36.086	19.459	1.00	31.89
1491	CA	ALA	A	207		19.203	34.651	19.541	1.00	30.97
1492	C	ALA	A	207		20.506	33.926	19.828	1.00	29.87
1493	O	ALA	A	207		20.485	32.707	20.028	1.00	30.21
1494	CB	ALA	A	207		18.657	34.153	18.183	1.00	30.74
1495	N	LEU	A	208		21.630	34.631	19.784	1.00	28.48
1496	CA	LEU	A	208		22.909	33.963	19.961	1.00	29.11
1497	C	LEU	A	208		23.516	34.215	21.336	1.00	29.38
1498	O	LEU	A	208		23.357	35.310	21.857	1.00	29.54
1499	CB	LEU	A	208		23.948	34.424	18.927	1.00	28.64
1500	CG	LEU	A	208		23.703	33.986	17.481	1.00	28.52
1501	CD1	LEU	A	208		24.704	34.659	16.558	1.00	27.66
1502	CD2	LEU	A	208		23.763	32.470	17.372	1.00	28.39
1503	N	SER	A	209		24.285	33.229	21.813	1.00	28.67
1504	CA	SER	A	209		24.999	33.395	23.072	1.00	27.73
1505	C	SER	A	209		26.090	34.453	22.903	1.00	27.76
1506	O	SER	A	209		26.493	34.797	21.800	1.00	26.99
1507	CB	SER	A	209		25.577	32.082	23.574	1.00	27.07
1508	OG	SER	A	209		26.481	32.291	24.653	1.00	26.06
1509	N	THR	A	210		26.482	35.063	24.008	1.00	29.62
1510	CA	THR	A	210		27.378	36.244	23.938	1.00	31.15
1511	C	THR	A	210		28.562	36.040	24.849	1.00	31.71
1512	O	THR	A	210		29.417	36.890	25.097	1.00	30.55

**FIG. 2-24C**

1513	CB	THR	A	210	26.495	37.458	24.255	1.00	31.98
1514	OG1	THR	A	210	26.238	38.187	23.037	1.00	32.30
1515	CG2	THR	A	210	27.039	38.393	25.302	1.00	32.74
1516	N	ARG	A	211	28.724	34.788	25.303	1.00	32.86
1517	CA	ARG	A	211	29.800	34.414	26.204	1.00	34.98
1518	C	ARG	A	211	31.142	34.331	25.505	1.00	35.34
1519	O	ARG	A	211	31.736	33.260	25.391	1.00	35.29
1520	CB	ARG	A	211	29.440	33.084	26.873	1.00	36.96
1521	CG	ARG	A	211	30.276	32.715	28.078	1.00	38.63
1522	CD	ARG	A	211	29.809	31.412	28.695	1.00	40.89
1523	NE	ARG	A	211	28.812	31.617	29.748	1.00	43.18
1524	CZ	ARG	A	211	27.497	31.538	29.556	1.00	44.37
1525	NH1	ARG	A	211	27.003	31.259	28.347	1.00	44.55
1526	NH2	ARG	A	211	26.676	31.740	30.581	1.00	44.44
1527	N	ASN	A	212	31.697	35.456	25.076	1.00	36.69
1528	CA	ASN	A	212	32.967	35.519	24.386	1.00	38.57
1529	C	ASN	A	212	34.172	35.285	25.283	1.00	40.78
1530	O	ASN	A	212	35.272	35.059	24.758	1.00	41.25
1531	CB	ASN	A	212	33.125	36.873	23.686	1.00	38.25
1532	CG	ASN	A	212	31.919	37.286	22.873	1.00	38.78
1533	OD1	ASN	A	212	31.326	36.500	22.126	1.00	38.93
1534	ND2	ASN	A	212	31.525	38.552	23.005	1.00	38.26

**FIG. 2-25A**

1535	N	ASP	A	213	34.018	35.328	26.601	1.00	43.10
1536	CA	ASP	A	213	35.130	35.122	27.525	1.00	45.40
1537	C	ASP	A	213	35.433	33.638	27.704	1.00	45.34
1538	O	ASP	A	213	36.540	33.257	28.080	1.00	44.99
1539	CB	ASP	A	213	34.896	35.821	28.858	1.00	47.21
1540	CG	ASP	A	213	33.652	35.405	29.603	1.00	49.21
1541	OD1	ASP	A	213	32.526	35.562	29.072	1.00	50.18
1542	OD2	ASP	A	213	33.789	34.906	30.749	1.00	50.24
1543	N	ASN	A	214	34.465	32.787	27.385	1.00	45.48
1544	CA	ASN	A	214	34.649	31.342	27.426	1.00	45.22
1545	C	ASN	A	214	33.840	30.670	26.316	1.00	43.77
1546	O	ASN	A	214	32.803	30.045	26.541	1.00	43.50
1547	CB	ASN	A	214	34.289	30.771	28.789	1.00	46.06
1548	CG	ASN	A	214	34.875	29.392	29.028	1.00	46.69
1549	OD1	ASN	A	214	35.114	29.005	30.174	1.00	47.37
1550	ND2	ASN	A	214	35.114	28.633	27.966	1.00	46.96
1551	N	PRO	A	215	34.345	30.763	25.089	1.00	42.47
1552	CA	PRO	A	215	33.653	30.271	23.911	1.00	41.85
1553	C	PRO	A	215	33.196	28.836	23.992	1.00	40.97
1554	O	PRO	A	215	32.078	28.509	23.586	1.00	40.92

**FIG. 2-25B**

1555	CB	PRO	A	215	34.665	30.467	22.785	1.00	41.51
1556	CG	PRO	A	215	35.519	31.597	23.234	1.00	41.27
1557	CD	PRO	A	215	35.569	31.517	24.730	1.00	41.71
1558	N	GLN	A	216	34.006	27.940	24.542	1.00	40.36
1559	CA	GLN	A	216	33.689	26.536	24.662	1.00	40.03
1560	C	GLN	A	216	32.649	26.243	25.736	1.00	38.52
1561	O	GLN	A	216	32.207	25.093	25.842	1.00	38.43
1562	CB	GLN	A	216	34.948	25.709	24.953	1.00	42.11
1563	CG	GLN	A	216	36.081	25.871	23.963	1.00	44.52
1564	CD	GLN	A	216	36.980	27.057	24.241	1.00	46.34
1565	OE1	GLN	A	216	36.910	27.707	25.293	1.00	47.64
1566	NE2	GLN	A	216	37.842	27.386	23.279	1.00	46.74
1567	N	ALA	A	217	32.268	27.225	26.536	1.00	36.20
1568	CA	ALA	A	217	31.303	27.017	27.608	1.00	34.50
1569	C	ALA	A	217	29.987	27.715	27.287	1.00	33.15
1570	O	ALA	A	217	28.997	27.578	28.001	1.00	32.25
1571	CB	ALA	A	217	31.880	27.557	28.914	1.00	34.14
1572	N	ALA	A	218	29.996	28.465	26.196	1.00	32.07
1573	CA	ALA	A	218	28.856	29.223	25.721	1.00	31.43
1574	C	ALA	A	218	27.613	28.361	25.529	1.00	31.15
1575	O	ALA	A	218	26.539	28.709	26.018	1.00	31.19

**FIG. 2-25C**

1576	CB	ALA	A	218	29.199	29.923	24.407	1.00	30.76
1577	N	SER	A	219	27.771	27.274	24.795	1.00	30.96
1578	CA	SER	A	219	26.679	26.362	24.487	1.00	31.23
1579	C	SER	A	219	26.385	25.476	25.684	1.00	31.50
1580	O	SER	A	219	27.187	24.600	26.008	1.00	30.63
1581	CB	SER	A	219	27.062	25.535	23.257	1.00	31.35
1582	OG	SER	A	219	25.973	24.795	22.745	1.00	31.74
1583	N	ARG	A	220	25.240	25.687	26.343	1.00	32.52
1584	CA	ARG	A	220	24.930	24.859	27.519	1.00	33.84
1585	C	ARG	A	220	23.463	24.496	27.638	1.00	34.32
1586	O	ARG	A	220	22.727	24.975	28.505	1.00	34.48
1587	CB	ARG	A	220	25.426	25.582	28.776	1.00	33.63
1588	CG	ARG	A	220	25.147	27.069	28.796	1.00	34.24
1589	CD	ARG	A	220	25.618	27.735	30.070	1.00	35.88
1590	NE	ARG	A	220	27.023	27.517	30.346	1.00	37.22
1591	CZ	ARG	A	220	27.541	26.815	31.336	1.00	37.40
1592	NH1	ARG	A	220	26.758	26.220	32.219	1.00	37.56
1593	NH2	ARG	A	220	28.863	26.708	31.450	1.00	38.33
1594	N	PRO	A	221	22.988	23.595	26.782	1.00	34.72
1595	CA	PRO	A	221	21.610	23.177	26.771	1.00	35.12
1596	C	PRO	A	221	21.070	22.782	28.127	1.00	36.33
1597	O	PRO	A	221	21.575	21.905	28.822	1.00	36.73
1598	CB	PRO	A	221	21.556	22.019	25.790	1.00	34.23

**FIG. 2-26A**



1599	CG	PRO	A	221	22.935	21.743	25.355	1.00	34.39
1600	CD	PRO	A	221	23.771	22.941	25.702	1.00	34.79
1601	N	TRP	A	222	19.982	23.430	28.537	1.00	37.81
1602	CA	TRP	A	222	19.253	23.204	29.764	1.00	38.35
1603	C	TRP	A	222	19.870	23.783	31.021	1.00	40.00
1604	O	TRP	A	222	19.244	23.803	32.087	1.00	40.39
1605	CB	TRP	A	222	18.989	21.704	29.960	1.00	37.21
1606	CG	TRP	A	222	18.017	21.170	28.940	1.00	36.16
1607	CD1	TRP	A	222	16.705	21.496	28.811	1.00	35.54
1608	CD2	TRP	A	222	18.304	20.213	27.913	1.00	35.39
1609	NE1	TRP	A	222	16.151	20.796	27.769	1.00	35.19
1610	CE2	TRP	A	222	17.111	20.004	27.203	1.00	35.06
1611	CE3	TRP	A	222	19.453	19.511	27.533	1.00	35.46
1612	CZ2	TRP	A	222	17.030	19.127	26.123	1.00	35.14
1613	CZ3	TRP	A	222	19.370	18.638	26.460	1.00	35.39
1614	CH2	TRP	A	222	18.165	18.456	25.770	1.00	35.07
1615	N	ASP	A	223	21.097	24.269	30.942	1.00	41.44
1616	CA	ASP	A	223	21.747	24.939	32.048	1.00	42.07

**FIG. 2-26B**



1639	OE1	GLU	A	225	26.658	31.171	34.461	1.00	52.70
1640	OE2	GLU	A	225	26.323	29.336	35.663	1.00	52.08
1641	N	ARG	A	226	22.030	29.558	30.316	1.00	42.31
1642	CA	ARG	A	226	21.854	29.621	28.870	1.00	40.38
1643	C	ARG	A	226	21.618	31.059	28.409	1.00	38.31
1644	O	ARG	A	226	20.851	31.766	29.076	1.00	38.79
1645	CB	ARG	A	226	20.595	28.839	28.463	1.00	41.11
1646	CG	ARG	A	226	20.733	27.358	28.276	1.00	42.80
1647	CD	ARG	A	226	19.386	26.645	28.252	1.00	44.07
1648	NE	ARG	A	226	18.414	27.281	29.116	1.00	46.50
1649	CZ	ARG	A	226	17.366	26.721	29.696	1.00	47.73
1650	NH1	ARG	A	226	17.078	25.440	29.522	1.00	48.79
1651	NH2	ARG	A	226	16.571	27.446	30.475	1.00	48.31
1652	N	ASP	A	227	22.171	31.480	27.286	1.00	36.03
1653	CA	ASP	A	227	21.891	32.830	26.791	1.00	33.63
1654	C	ASP	A	227	21.674	32.838	25.285	1.00	32.31
1655	O	ASP	A	227	21.554	33.919	24.700	1.00	32.59
1656	CB	ASP	A	227	22.967	33.825	27.192	1.00	32.84
1657	CG	ASP	A	227	24.334	33.499	26.637	1.00	33.33
1658	OD1	ASP	A	227	24.627	32.286	26.529	1.00	34.69
1659	OD2	ASP	A	227	25.120	34.414	26.307	1.00	32.44

**FIG. 2-27A**

1660	N	GLY	A	228			21.550	31.672	24.654	1.00	30.62
1661	CA	GLY	A	228			21.366	31.677	23.188	1.00	28.87
1662	C	GLY	A	228			22.125	30.526	22.548	1.00	27.72
1663	O	GLY	A	228			23.023	29.955	23.172	1.00	28.88
1664	N	PHE	A	229			21.754	30.147	21.330	1.00	25.72
1665	CA	PHE	A	229			22.412	29.027	20.666	1.00	22.79
1666	C	PHE	A	229			23.772	29.488	20.159	1.00	22.85
1667	O	PHE	A	229			24.077	30.672	20.162	1.00	21.95
1668	CB	PHE	A	229			21.550	28.413	19.591	1.00	21.43
1669	CG	PHE	A	229			21.327	29.142	18.316	1.00	20.46
1670	CD1	PHE	A	229			22.236	29.069	17.275	1.00	19.91
1671	CD2	PHE	A	229			20.191	29.920	18.131	1.00	20.66
1672	CE1	PHE	A	229			22.025	29.759	16.087	1.00	19.15
1673	CE2	PHE	A	229			19.969	30.605	16.944	1.00	19.34
1674	CZ	PHE	A	229			20.894	30.517	15.928	1.00	18.75
1675	N	VAL	A	230			24.597	28.526	19.795	1.00	24.11
1676	CA	VAL	A	230			25.926	28.768	19.252	1.00	24.59
1677	C	VAL	A	230			25.972	28.253	17.810	1.00	24.91
1678	O	VAL	A	230			25.540	27.150	17.497	1.00	23.86
1679	CB	VAL	A	230			27.024	28.118	20.106	1.00	24.60

**FIG. 2-27B**

1680	CG1	VAL	A	230		28.392	28.206	19.448	1.00	23.60
1681	CG2	VAL	A	230		27.076	28.781	21.486	1.00	23.95
1682	N	LEU	A	231		26.347	29.141	16.910	1.00	26.19
1683	CA	LEU	A	231		26.347	28.898	15.471	1.00	27.19
1684	C	LEU	A	231		27.458	27.932	15.080	1.00	27.61
1685	O	LEU	A	231		28.575	28.038	15.608	1.00	27.83
1686	CB	LEU	A	231		26.532	30.244	14.786	1.00	27.96
1687	CG	LEU	A	231		26.207	30.468	13.329	1.00	29.21
1688	CD1	LEU	A	231		25.563	29.269	12.659	1.00	29.75
1689	CD2	LEU	A	231		25.315	31.702	13.176	1.00	29.24
1690	N	GLY	A	232		27.171	27.010	14.159	1.00	26.20
1691	CA	GLY	A	232		28.192	26.067	13.714	1.00	24.72
1692	C	GLY	A	232		28.023	25.702	12.248	1.00	23.99
1693	O	GLY	A	232		26.901	25.451	11.800	1.00	24.18
1694	N	ASP	A	233		29.117	25.550	11.512	1.00	23.28
1695	CA	ASP	A	233		29.061	25.134	10.117	1.00	22.60
1696	C	ASP	A	233		29.340	23.637	9.959	1.00	21.54
1697	O	ASP	A	233		29.988	23.027	10.810	1.00	20.87
1698	CB	ASP	A	233		30.079	25.883	9.261	1.00	23.15
1699	CG	ASP	A	233		30.103	27.370	9.485	1.00	24.40
1700	OD1	ASP	A	233		29.054	27.994	9.749	1.00	24.44
1701	OD2	ASP	A	233		31.216	27.933	9.398	1.00	26.06

**FIG. 2-27C**

1702	N	GLY	A	234	28.918	23.080	8.825	1.00	20.29
1703	CA	GLY	A	234	29.210	21.686	8.549	1.00	21.48
1704	C	GLY	A	234	28.252	21.018	7.587	1.00	22.09
1705	O	GLY	A	234	27.397	21.642	6.971	1.00	22.10
1706	N	ALA	A	235	28.367	19.694	7.476	1.00	23.04
1707	CA	ALA	A	235	27.488	18.924	6.612	1.00	24.26
1708	C	ALA	A	235	27.550	17.452	7.013	1.00	25.10
1709	O	ALA	A	235	28.601	16.959	7.413	1.00	25.69
1710	CB	ALA	A	235	27.839	19.064	5.141	1.00	24.12
1711	N	GLY	A	236	26.406	16.810	6.904	1.00	25.31
1712	CA	GLY	A	236	26.263	15.399	7.203	1.00	25.96
1713	C	GLY	A	236	25.401	14.764	6.106	1.00	27.84
1714	O	GLY	A	236	24.292	15.232	5.828	1.00	28.18
1715	N	MET	A	237	25.956	13.732	5.480	1.00	27.94
1716	CA	MET	A	237	25.264	13.032	4.412	1.00	28.58
1717	C	MET	A	237	25.021	11.579	4.791	1.00	29.18
1718	O	MET	A	237	25.840	10.946	5.457	1.00	30.25
1719	CB	MET	A	237	26.058	13.121	3.111	1.00	29.09
1720	CG	MET	A	237	26.241	14.540	2.584	1.00	30.84
1721	SD	MET	A	237	24.689	15.275	2.005	1.00	31.49
1722	CE	MET	A	237	23.983	13.854	1.197	1.00	32.58

**FIG. 2-28A**

1723	N	LEU	A	238	23.861	11.059	4.432	1.00	29.03
1724	CA	LEU	A	238	23.455	9.697	4.647	1.00	28.93
1725	C	LEU	A	238	23.154	9.058	3.274	1.00	30.08
1726	O	LEU	A	238	22.641	9.736	2.395	1.00	30.53
1727	CB	LEU	A	238	22.174	9.573	5.445	1.00	29.18
1728	CG	LEU	A	238	21.953	9.963	6.879	1.00	28.28
1729	CD1	LEU	A	238	21.343	8.806	7.674	1.00	28.10
1730	CD2	LEU	A	238	23.203	10.416	7.588	1.00	28.92
1731	N	VAL	A	239	23.389	7.769	3.139	1.00	31.20
1732	CA	VAL	A	239	22.950	7.027	1.966	1.00	31.08
1733	C	VAL	A	239	21.801	6.122	2.442	1.00	31.88
1734	O	VAL	A	239	21.972	5.326	3.365	1.00	31.48
1735	CB	VAL	A	239	24.047	6.189	1.317	1.00	30.98
1736	CG1	VAL	A	239	23.493	5.297	0.207	1.00	30.65
1737	CG2	VAL	A	239	25.150	7.069	0.756	1.00	30.59
1738	N	LEU	A	240	20.614	6.367	1.910	1.00	32.81
1739	CA	LEU	A	240	19.465	5.539	2.267	1.00	34.06
1740	C	LEU	A	240	19.197	4.602	1.091	1.00	35.24
1741	O	LEU	A	240	19.377	5.025	-0.056	1.00	35.94

**FIG. 2-28B**

1742	CB	LEU	A	240	18.233	6.367	2.568	1.00	34.52
1743	CG	LEU	A	240	18.327	7.391	3.694	1.00	34.89
1744	CD1	LEU	A	240	17.392	8.562	3.424	1.00	35.01
1745	CD2	LEU	A	240	18.007	6.741	5.029	1.00	34.67
1746	N	GLU	A	241	18.858	3.355	1.376	1.00	36.34
1747	CA	GLU	A	241	18.549	2.426	0.288	1.00	37.40
1748	C	GLU	A	241	17.604	1.337	0.790	1.00	38.22
1749	O	GLU	A	241	17.459	1.156	1.997	1.00	37.42
1750	CB	GLU	A	241	19.775	1.860	-0.376	1.00	37.02
1751	CG	GLU	A	241	20.414	0.626	0.198	1.00	36.23
1752	CD	GLU	A	241	21.624	0.198	-0.629	1.00	36.50
1753	OE1	GLU	A	241	22.743	0.616	-0.277	1.00	36.26
1754	OE2	GLU	A	241	21.457	-0.538	-1.624	1.00	36.05
1755	N	GLU	A	242	16.839	0.808	-0.161	1.00	39.24
1756	CA	GLU	A	242	15.825	-0.196	0.151	1.00	40.59
1757	C	GLU	A	242	16.502	-1.471	0.625	1.00	42.13
1758	O	GLU	A	242	17.499	-1.913	0.049	1.00	42.65
1759	CB	GLU	A	242	14.947	-0.425	-1.073	1.00	40.67
1760	CG	GLU	A	242	13.767	-1.365	-0.852	1.00	40.14
1761	CD	GLU	A	242	14.158	-2.796	-1.182	1.00	40.03
1762	OE1	GLU	A	242	15.061	-2.964	-2.033	1.00	40.30
1763	OE2	GLU	A	242	13.583	-3.715	-0.577	1.00	40.12
1764	N	TYR	A	243	15.985	-2.050	1.688	1.00	44.48

**FIG. 2-28C**



1765	CA	TYR	A	243	16.528	-3.249	2.295	1.00	47.55
1766	C	TYR	A	243	16.969	-4.314	1.312	1.00	49.06
1767	O	TYR	A	243	18.165	-4.612	1.194	1.00	48.62
1768	CB	TYR	A	243	15.501	-3.828	3.281	1.00	49.37
1769	CG	TYR	A	243	16.082	-4.940	4.129	1.00	51.38
1770	CD1	TYR	A	243	16.964	-4.671	5.162	1.00	51.69
1771	CD2	TYR	A	243	15.741	-6.264	3.873	1.00	52.26
1772	CE1	TYR	A	243	17.492	-5.698	5.921	1.00	52.76
1773	CE2	TYR	A	243	16.261	-7.293	4.635	1.00	52.69
1774	CZ	TYR	A	243	17.141	-7.004	5.652	1.00	52.88
1775	OH	TYR	A	243	17.668	-8.024	6.409	1.00	53.60
1776	N	GLU	A	244	16.023	-4.912	0.584	1.00	50.65
1777	CA	GLU	A	244	16.323	-5.960	-0.383	1.00	51.25
1778	C	GLU	A	244	17.448	-5.559	-1.325	1.00	51.58
1779	O	GLU	A	244	18.371	-6.345	-1.534	1.00	51.59
1780	CB	GLU	A	244	15.091	-6.361	-1.191	1.00	51.54
1781	CG	GLU	A	244	13.925	-6.882	-0.386	1.00	52.35
1782	CD	GLU	A	244	14.242	-8.097	0.454	1.00	53.32
1783	OE1	GLU	A	244	15.188	-8.845	0.125	1.00	53.91
1784	OE2	GLU	A	244	13.535	-8.312	1.464	1.00	53.96
1785	N	HIS	A	245	17.376	-4.358	-1.889	1.00	52.37
1786	CA	HIS	A	245	18.422	-3.872	-2.788	1.00	53.53

**FIG. 2-29A**

1787	C	HIS	A	245	19.776	-3.940	-2.079	1.00	54.72
1788	O	HIS	A	245	20.741	-4.460	-2.619	1.00	54.26
1789	CB	HIS	A	245	18.120	-2.454	-3.239	1.00	53.08
1790	CG	HIS	A	245	19.042	-1.894	-4.277	1.00	52.59
1791	ND1	HIS	A	245	20.337	-1.511	-4.003	1.00	52.62
1792	CD2	HIS	A	245	18.841	-1.610	-5.584	1.00	52.43
1793	CE1	HIS	A	245	20.899	-1.032	-5.096	1.00	52.61
1794	NE2	HIS	A	245	20.012	-1.087	-6.075	1.00	52.66
1795	N	ALA	A	246	19.814	-3.419	-0.859	1.00	56.49
1796	CA	ALA	A	246	20.984	-3.410	-0.006	1.00	58.02
1797	C	ALA	A	246	21.414	-4.832	0.362	1.00	59.33
1798	O	ALA	A	246	22.605	-5.134	0.342	1.00	59.12
1799	CB	ALA	A	246	20.685	-2.632	1.276	1.00	57.55
1800	N	LYS	A	247	20.452	-5.691	0.677	1.00	60.88
1801	CA	LYS	A	247	20.736	-7.079	1.017	1.00	62.53
1802	C	LYS	A	247	21.478	-7.785	-0.112	1.00	63.46
1803	C	LYS	A	247	22.586	-8.299	0.062	1.00	64.16
1804	CB	LYS	A	247	19.444	-7.828	1.336	1.00	62.93
1805	CG	LYS	A	247	19.190	-8.093	2.806	1.00	63.75

**FIG. 2-29B**

1806	CD	LYS	A	247	18.323	-9.329	3.008	1.00	64.65
1807	CE	LYS	A	247	18.834	-10.207	4.137	1.00	65.11
1808	NZ	LYS	A	247	17.770	-11.078	4.710	1.00	65.33
1809	N	LYS	A	248	20.890	-7.806	-1.300	1.00	63.98
1810	CA	LYS	A	248	21.459	-8.440	-2.475	1.00	64.52
1811	C	LYS	A	248	22.870	-7.995	-2.808	1.00	64.22
1812	O	LYS	A	248	23.676	-8.794	-3.305	1.00	64.61
1813	CB	LYS	A	248	20.526	-8.201	-3.673	1.00	65.73
1814	CG	LYS	A	248	21.041	-8.731	-4.997	1.00	67.49
1815	CD	LYS	A	248	19.933	-9.335	-5.847	1.00	68.99
1816	CE	LYS	A	248	19.422	-10.650	-5.279	1.00	69.64
1817	NZ	LYS	A	248	18.013	-10.943	-5.671	1.00	69.80
1818	N	ARG	A	249	23.220	-6.740	-2.582	1.00	63.72
1819	CA	ARG	A	249	24.542	-6.222	-2.893	1.00	63.29
1820	C	ARG	A	249	25.520	-6.419	-1.743	1.00	62.36
1821	O	ARG	A	249	26.712	-6.136	-1.891	1.00	62.39
1822	CB	ARG	A	249	24.449	-4.730	-3.260	1.00	63.82
1823	CG	ARG	A	249	23.678	-3.920	-2.231	1.00	64.36
1824	CD	ARG	A	249	23.874	-2.430	-2.376	1.00	64.71
1825	NE	ARG	A	249	25.279	-2.056	-2.335	1.00	64.93
1826	CZ	ARG	A	249	25.762	-0.961	-1.772	1.00	64.91
1827	NH1	ARG	A	249	24.951	-0.101	-1.182	1.00	64.78

**FIG. 2-29C**

1828	NH2	ARG	A	249	27.067	-0.745	-1.812	1.00	65.38
1829	N	GLY	A	250	25.040	-6.911	-0.607	1.00	60.87
1830	CA	GLY	A	250	25.913	-7.131	0.548	1.00	59.90
1831	C	GLY	A	250	26.469	-5.794	1.037	1.00	58.77
1832	O	GLY	A	250	27.666	-5.532	0.986	1.00	58.78
1833	N	ALA	A	251	25.565	-4.945	1.522	1.00	57.41
1834	CA	ALA	A	251	25.944	-3.621	1.977	1.00	55.66
1835	C	ALA	A	251	26.096	-3.568	3.491	1.00	54.72
1836	O	ALA	A	251	25.302	-4.138	4.231	1.00	55.01
1837	CB	ALA	A	251	24.901	-2.602	1.531	1.00	55.46
1838	N	LYS	A	252	27.088	-2.814	3.936	1.00	53.10
1839	CA	LYS	A	252	27.217	-2.428	5.336	1.00	51.33
1840	C	LYS	A	252	25.891	-1.818	5.792	1.00	49.96
1841	O	LYS	A	252	25.612	-0.691	5.346	1.00	50.79
1842	CB	LYS	A	252	28.294	-1.349	5.418	1.00	51.97
1843	CG	LYS	A	252	29.460	-1.544	6.340	1.00	52.61
1844	CD	LYS	A	252	30.208	-0.239	6.593	1.00	53.01
1845	CE	LYS	A	252	30.836	0.346	5.343	1.00	52.98
1846	NZ	LYS	A	252	32.219	-0.157	5.097	1.00	53.69
1847	N	ILE	A	253	25.090	-2.482	6.604	1.00	47.12
1848	CA	ILE	A	253	23.840	-1.881	7.062	1.00	44.71
1849	C	ILE	A	253	24.020	-1.246	8.435	1.00	43.36

**FIG. 2-30A**

1850	O	ILE	A	253	24.012	-1.935	9.462	1.00	44.22
1851	CB	ILE	A	253	22.674	-2.884	7.110	1.00	45.09
1852	CG1	ILE	A	253	22.284	-3.326	5.694	1.00	44.84
1853	CG2	ILE	A	253	21.477	-2.282	7.844	1.00	44.25
1854	CD1	ILE	A	253	20.932	-4.007	5.591	1.00	44.67
1855	N	TYR	A	254	24.049	0.082	8.495	1.00	41.00
1856	CA	TYR	A	254	24.201	0.773	9.772	1.00	38.50
1857	C	TYR	A	254	22.948	0.731	10.628	1.00	37.38
1858	O	TYR	A	254	23.010	0.615	11.853	1.00	38.15
1859	CB	TYR	A	254	24.571	2.235	9.557	1.00	37.33
1860	CG	TYR	A	254	25.979	2.477	9.071	1.00	36.11
1861	CD1	TYR	A	254	26.250	2.657	7.726	1.00	35.30
1862	CD2	TYR	A	254	27.031	2.550	9.972	1.00	35.51
1863	CE1	TYR	A	254	27.538	2.899	7.292	1.00	35.59
1864	CE2	TYR	A	254	28.322	2.787	9.545	1.00	34.81
1865	CZ	TYR	A	254	28.567	2.969	8.209	1.00	35.14
1866	OH	TYR	A	254	29.845	3.209	7.764	1.00	35.01
1867	N	ALA	A	255	21.792	0.886	10.004	1.00	36.44

**FIG. 2-30B**

1868	CA	ALA	A	255		20.536	0.899	10.748	1.00	35.71
1869	C	ALA	A	255		19.367	0.917	9.769	1.00	35.68
1870	O	ALA	A	255		19.573	0.959	8.558	1.00	34.91
1871	CB	ALA	A	255		20.481	2.114	11.662	1.00	35.22
1872	N	GLU	A	256		18.168	0.899	10.321	1.00	36.53
1873	CA	GLU	A	256		16.945	0.951	9.552	1.00	37.42
1874	C	GLU	A	256		16.152	2.209	9.902	1.00	37.04
1875	O	GLU	A	256		15.941	2.490	11.086	1.00	36.85
1876	CB	GLU	A	256		16.054	-0.267	9.831	1.00	39.31
1877	CG	GLU	A	256		15.103	-0.594	8.690	1.00	42.01
1878	CD	GLU	A	256		14.074	-1.643	9.048	1.00	43.86
1879	OE1	GLU	A	256		12.853	-1.395	8.910	1.00	44.65
1880	OE2	GLU	A	256		14.479	-2.750	9.478	1.00	45.17
1881	N	LEU	A	257		15.723	2.931	8.874	1.00	36.43
1882	CA	LEU	A	257		14.882	4.120	9.112	1.00	35.83
1883	C	LEU	A	257		13.456	3.603	9.292	1.00	35.09
1884	O	LEU	A	257		12.950	2.950	8.368	1.00	35.81
1885	CB	LEU	A	257		14.990	5.075	7.952	1.00	36.17
1886	CG	LEU	A	257		14.474	6.497	8.023	1.00	36.62
1887	CD1	LEU	A	257		14.176	6.980	9.428	1.00	36.47
1888	CD2	LEU	A	257		15.503	7.434	7.371	1.00	36.59
1889	N	VAL	A	258		12.898	3.663	10.496	1.00	34.38
1890	CA	VAL	A	258		11.603	3.034	10.719	1.00	34.14

**FIG. 2-30C**

1891	C	VAL	A	258	10.495	4.012	11.049	1.00	33.65
1892	O	VAL	A	258	9.349	3.561	11.194	1.00	34.38
1893	CB	VAL	A	258	11.619	1.965	11.845	1.00	34.54
1894	CG1	VAL	A	258	12.689	0.913	11.602	1.00	33.95
1895	CG2	VAL	A	258	11.761	2.594	13.219	1.00	32.70
1896	N	GLY	A	259	10.787	5.287	11.243	1.00	33.01
1897	CA	GLY	A	259	9.718	6.223	11.594	1.00	32.64
1898	C	GLY	A	259	10.094	7.640	11.195	1.00	33.38
1899	O	GLY	A	259	11.260	8.010	11.307	1.00	34.33
1900	N	PHE	A	260	9.104	8.408	10.758	1.00	32.82
1901	CA	PHE	A	260	9.288	9.793	10.342	1.00	31.11
1902	C	PHE	A	260	8.028	10.607	10.608	1.00	30.38
1903	O	PHE	A	260	6.958	10.321	10.062	1.00	30.80
1904	CB	PHE	A	260	9.666	9.859	8.864	1.00	30.74
1905	CG	PHE	A	260	9.673	11.244	8.289	1.00	30.39
1906	CD1	PHE	A	260	10.339	12.272	8.939	1.00	30.56
1907	CD2	PHE	A	260	9.014	11.518	7.103	1.00	30.06
1908	CE1	PHE	A	260	10.344	13.552	8.419	1.00	30.43
1909	CE2	PHE	A	260	9.023	12.791	6.566	1.00	29.90
1910	CZ	PHE	A	260	9.687	13.803	7.227	1.00	30.57
1911	N	GLY	A	261	8.141	11.610	11.470	1.00	29.70
1912	CA	GLY	A	261	7.008	12.434	11.837	1.00	28.92
1913	C	GLY	A	261	7.223	13.919	11.616	1.00	29.15

**FIG. 2-31A**

1914	O	GLY	A		261	8.264	14.502	11.927	1.00	28.06
1915	N	MET	A		262	6.195	14.568	11.075	1.00	29.65
1916	CA	MET	A		262	6.234	16.006	10.832	1.00	30.20
1917	C	MET	A		262	5.070	16.647	11.596	1.00	30.06
1918	O	MET	A		262	4.076	15.969	11.820	1.00	30.13
1919	CB	MET	A		262	6.108	16.345	9.363	1.00	30.45
1920	CG	MET	A		262	7.201	15.870	8.440	1.00	30.83
1921	SD	MET	A		262	6.528	15.370	6.839	1.00	33.07
1922	CE	MET	A		262	6.552	16.931	5.973	1.00	33.59
1923	N	SER	A		263	5.220	17.898	11.968	1.00	30.55
1924	CA	SER	A		263	4.195	18.630	12.684	1.00	31.14
1925	C	SER	A		263	4.371	20.143	12.513	1.00	31.88
1926	O	SER	A		263	5.461	20.618	12.178	1.00	31.41
1927	CB	SER	A		263	4.271	18.315	14.184	1.00	31.36
1928	OG	SER	A		263	5.026	19.356	14.817	1.00	32.23
1929	N	SER	A		264	3.304	20.883	12.800	1.00	32.27
1930	CA	SER	A		264	3.383	22.344	12.751	1.00	33.13
1931	C	SER	A		264	2.953	22.913	14.107	1.00	33.50

**FIG. 2-31B**



1932	O	SER	A	264	2.190	22.277	14.843	1.00	34.89
1933	CB	SER	A	264	2.563	22.928	11.619	1.00	33.19
1934	OG	SER	A	264	3.245	22.889	10.378	1.00	32.30
1935	N	ASP	A	265	3.549	24.024	14.495	1.00	32.03
1936	CA	ASP	A	265	3.310	24.635	15.783	1.00	31.81
1937	C	ASP	A	265	2.084	25.546	15.757	1.00	33.26
1938	O	ASP	A	265	1.225	25.499	16.637	1.00	33.79
1939	CB	ASP	A	265	4.523	25.457	16.231	1.00	29.59
1940	CG	ASP	A	265	5.554	24.701	17.034	1.00	27.79
1941	OD1	ASP	A	265	5.426	23.486	17.253	1.00	25.02
1942	OD2	ASP	A	265	6.556	25.343	17.450	1.00	27.38
1943	N	ALA	A	266	2.039	26.413	14.753	1.00	34.80
1944	CA	ALA	A	266	0.929	27.352	14.616	1.00	36.45
1945	C	ALA	A	266	0.882	28.274	15.829	1.00	38.12
1946	O	ALA	A	266	-0.183	28.542	16.390	1.00	39.22
1947	CB	ALA	A	266	-0.366	26.578	14.412	1.00	35.63
1948	N	TYR	A	267	2.047	28.804	16.209	1.00	39.02
1949	CA	TYR	A	267	2.138	29.676	17.365	1.00	40.82
1950	C	TYR	A	267	2.858	30.985	17.074	1.00	40.11
1951	O	TYR	A	267	2.279	32.071	17.056	1.00	40.09
1952	CB	TYR	A	267	2.853	28.938	18.513	1.00	42.94
1953	CG	TYR	A	267	2.995	29.795	19.754	1.00	45.78

**FIG. 2-31C**

1954	CD1	TYR	A	267	1.870	30.187	20.475	1.00	46.70
1955	CD2	TYR	A	267	4.240	30.225	20.194	1.00	46.17
1956	CE1	TYR	A	267	1.997	30.980	21.598	1.00	47.78
1957	CE2	TYR	A	267	4.369	31.016	21.316	1.00	46.66
1958	CZ	TYR	A	267	3.246	31.393	22.012	1.00	47.81
1959	OH	TYR	A	267	3.352	32.177	23.146	1.00	49.51
1960	N	HIS	A	268	4.167	30.890	16.898	1.00	39.39
1961	CA	HIS	A	268	4.985	32.066	16.641	1.00	38.82
1962	C	HIS	A	268	5.976	31.797	15.519	1.00	38.25
1963	O	HIS	A	268	6.275	30.640	15.227	1.00	37.62
1964	CB	HIS	A	268	5.684	32.479	17.942	1.00	38.89
1965	CG	HIS	A	268	6.302	33.838	17.821	1.00	38.92
1966	ND1	HIS	A	268	7.602	34.018	17.404	1.00	39.06
1967	CD2	HIS	A	268	5.784	35.065	18.025	1.00	39.28
1968	CE1	HIS	A	268	7.871	35.309	17.376	1.00	39.76
1969	NE2	HIS	A	268	6.783	35.966	17.743	1.00	40.01
1970	N	MET	A	269	6.475	32.851	14.890	1.00	38.43
1971	CA	MET	A	269	7.351	32.732	13.739	1.00	39.01
1972	C	MET	A	269	8.749	32.275	14.107	1.00	39.15
1973	O	MET	A	269	9.426	31.657	13.275	1.00	39.25
1974	CB	MET	A	269	7.386	34.016	12.910	1.00	38.43
1975	CG	MET	A	269	7.675	35.291	13.655	1.00	38.54

**FIG. 2-32A**

1976	SD	MET	A	269				8.284	36.624	12.597	1.00	39.05
1977	CE	MET	A	269				6.747	37.295	11.973	1.00	38.85
1978	N	THR	A	270				9.206	32.554	15.318	1.00	39.79
1979	CA	THR	A	270				10.544	32.142	15.738	1.00	39.79
1980	C	THR	A	270				10.491	31.386	17.061	1.00	39.73
1981	O	THR	A	270				11.262	30.461	17.286	1.00	40.16
1982	CB	THR	A	270				11.500	33.336	15.909	1.00	39.47
1983	OG1	THR	A	270				10.849	34.378	16.650	1.00	38.86
1984	CG2	THR	A	270				11.946	33.850	14.549	1.00	39.41
1985	N	SER	A	271				9.562	31.784	17.912	1.00	39.92
1986	CA	SER	A	271				9.368	31.191	19.218	1.00	40.15
1987	C	SER	A	271				8.529	29.923	19.208	1.00	39.41
1988	O	SER	A	271				7.519	29.833	18.522	1.00	38.39
1989	CB	SER	A	271				8.655	32.218	20.122	1.00	40.93
1990	OG	SER	A	271				9.597	32.892	20.930	1.00	42.94
1991	N	PRO	A	272				8.916	28.967	20.033	1.00	39.55
1992	CA	PRO	A	272				8.149	27.755	20.264	1.00	39.89
1993	C	PRO	A	272				7.144	27.989	21.382	1.00	40.70
1994	O	PRO	A	272				7.253	28.945	22.155	1.00	40.74
1995	CB	PRO	A	272				9.213	26.763	20.710	1.00	39.54

**FIG. 2-32B**

1996	CG	PRO	A	272	10.251	27.585	21.378	1.00	39.69
1997	CD	PRO	A	272	10.104	29.011	20.924	1.00	39.50
1998	N	PRO	A	273	6.128	27.155	21.451	1.00	41.57
1999	CA	PRO	A	273	5.155	27.209	22.529	1.00	41.97
2000	C	PRO	A	273	5.763	26.687	23.815	1.00	42.79
2001	O	PRO	A	273	6.367	25.604	23.834	1.00	42.22
2002	CB	PRO	A	273	4.021	26.336	22.032	1.00	41.91
2003	CG	PRO	A	273	4.442	25.701	20.769	1.00	41.49
2004	CD	PRO	A	273	5.908	25.976	20.573	1.00	41.55
2005	N	GLU	A	274	5.557	27.355	24.947	1.00	44.77
2006	CA	GLU	A	274	6.113	26.899	26.229	1.00	46.56
2007	C	GLU	A	274	5.820	25.427	26.481	1.00	45.89
2008	O	GLU	A	274	6.614	24.681	27.049	1.00	46.05
2009	CB	GLU	A	274	5.598	27.763	27.382	1.00	48.17
2010	CG	GLU	A	274	6.173	29.169	27.404	1.00	49.92
2011	CD	GLU	A	274	6.416	29.712	28.793	1.00	51.48
2012	OE1	GLU	A	274	5.443	30.190	29.421	1.00	52.14
2013	OE2	GLU	A	274	7.573	29.677	29.280	1.00	52.45
2014	N	ASN	A	275	4.655	24.997	26.094	1.00	45.72
2015	CA	ASN	A	275	4.102	23.686	26.059	1.00	46.22
2016	C	ASN	A	275	4.974	22.643	25.375	1.00	45.27

**FIG. 2-32C**

2017	O	ASN	A	275	5.181	21.540	25.870	1.00	45.50
2018	CB	ASN	A	275	2.792	23.832	25.226	1.00	48.36
2019	CG	ASN	A	275	1.786	22.757	25.501	1.00	50.56
2020	ODI	ASN	A	275	0.610	23.052	25.746	1.00	51.89
2021	ND2	ASN	A	275	2.222	21.499	25.461	1.00	51.68
2022	N	GLY	A	276	5.404	22.926	24.142	1.00	43.78
2023	CA	GLY	A	276	6.162	21.984	23.332	1.00	41.18
2024	C	GLY	A	276	5.229	21.052	22.558	1.00	39.94
2025	O	GLY	A	276	5.630	19.999	22.057	1.00	38.60
2026	N	ALA	A	277	3.960	21.444	22.429	1.00	38.88
2027	CA	ALA	A	277	2.943	20.651	21.765	1.00	38.13
2028	C	ALA	A	277	3.282	20.243	20.338	1.00	37.49
2029	O	ALA	A	277	2.921	19.138	19.911	1.00	37.45
2030	CB	ALA	A	277	1.602	21.380	21.780	1.00	37.64
2031	N	GLY	A	278	3.871	21.144	19.562	1.00	36.32
2032	CA	GLY	A	278	4.257	20.831	18.183	1.00	34.59
2033	C	GLY	A	278	5.357	19.776	18.211	1.00	33.11
2034	O	GLY	A	278	5.263	18.743	17.545	1.00	32.66
2035	N	ALA	A	279	6.362	20.011	19.051	1.00	31.37
2036	CA	ALA	A	279	7.431	19.025	19.215	1.00	31.33
2037	C	ALA	A	279	6.857	17.681	19.660	1.00	31.17
2038	O	ALA	A	279	7.231	16.611	19.159	1.00	31.33

**FIG. 2-33A**

2039	CB	ALA	A	279		8.444	19.546	20.212	1.00	31.56
2040	N	ALA	A	280		5.884	17.714	20.562	1.00	30.93
2041	CA	ALA	A	280		5.212	16.518	21.041	1.00	31.18
2042	C	ALA	A	280		4.505	15.758	19.932	1.00	31.56
2043	O	ALA	A	280		4.626	14.536	19.788	1.00	31.58
2044	CB	ALA	A	280		4.227	16.911	22.141	1.00	30.59
2045	N	LEU	A	281		3.781	16.482	19.078	1.00	31.84
2046	CA	LEU	A	281		2.989	15.831	18.031	1.00	32.50
2047	C	LEU	A	281		3.840	15.238	16.924	1.00	32.77
2048	O	LEU	A	281		3.402	14.330	16.205	1.00	32.06
2049	CB	LEU	A	281		1.958	16.823	17.508	1.00	33.11
2050	CG	LEU	A	281		1.157	16.429	16.271	1.00	34.64
2051	CD1	LEU	A	281		0.256	15.241	16.556	1.00	33.87
2052	CD2	LEU	A	281		0.351	17.623	15.767	1.00	34.77
2053	N	ALA	A	282		5.072	15.723	16.774	1.00	32.69
2054	CA	ALA	A	282		5.988	15.209	15.765	1.00	31.83
2055	C	ALA	A	282		6.667	13.936	16.256	1.00	31.20
2056	O	ALA	A	282		6.953	13.060	15.448	1.00	29.68
2057	CB	ALA	A	282		7.022	16.256	15.397	1.00	32.01

**FIG. 2-33B**

2058	N	MET	A	283			6.927		13.865	17.571	1.00	31.55
2059	CA	MET	A	283			7.522		12.619	18.101	1.00	32.09
2060	C	MET	A	283			6.415		11.558	18.038	1.00	32.78
2061	O	MET	A	283			6.510		10.526	17.386	1.00	32.13
2062	CB	MET	A	283			8.041		12.793	19.507	1.00	31.89
2063	CG	MET	A	283			9.262		13.684	19.646	1.00	31.94
2064	SD	MET	A	283			9.783		13.914	21.342	1.00	31.98
2065	CE	MET	A	283			8.955		15.399	21.846	1.00	31.11
2066	N	ALA	A	284			5.274		11.947	18.604	1.00	33.35
2067	CA	ALA	A	284			4.038		11.207	18.566	1.00	33.77
2068	C	ALA	A	284			3.757		10.601	17.196	1.00	34.98
2069	O	ALA	A	284			3.547		9.387	17.080	1.00	36.92
2070	CB	ALA	A	284			2.907		12.160	18.950	1.00	33.34
2071	N	ASN	A	285			3.789		11.409	16.147	1.00	35.09
2072	CA	ASN	A	285			3.535		10.975	14.782	1.00	34.98
2073	C	ASN	A	285			4.601		10.009	14.281	1.00	35.26
2074	O	ASN	A	285			4.339		9.059	13.540	1.00	35.45
2075	CB	ASN	A	285			3.433		12.196	13.863	1.00	34.80
2076	CG	ASN	A	285			2.128		12.946	13.906	1.00	35.23
2077	OD1	ASN	A	285			1.075		12.436	14.290	1.00	36.24
2078	ND2	ASN	A	285			2.126		14.219	13.505	1.00	34.94
2079	N	ALA	A	286			5.854		10.220	14.671	1.00	35.27

**FIG. 2-33C**

2080	CA	ALA	A	286		6.964	9.362	14.285	1.00	34.55
2081	C	ALA	A	286		6.742	7.970	14.874	1.00	35.42
2082	O	ALA	A	286		6.960	6.935	14.264	1.00	34.04
2083	CB	ALA	A	286		8.268	9.936	14.818	1.00	33.75
2084	N	LEU	A	287		6.321	7.995	16.143	1.00	37.17
2085	CA	LEU	A	287		6.018	6.780	16.884	1.00	38.32
2086	C	LEU	A	287		4.957	5.967	16.164	1.00	39.73
2087	O	LEU	A	287		5.158	4.784	15.877	1.00	38.69
2088	CB	LEU	A	287		5.600	7.154	18.313	1.00	37.88
2089	CG	LEU	A	287		6.795	7.426	19.249	1.00	37.80
2090	CD1	LEU	A	287		6.334	7.877	20.616	1.00	37.05
2091	CD2	LEU	A	287		7.683	6.190	19.347	1.00	37.58
2092	N	ARG	A	288		3.851	6.632	15.806	1.00	41.38
2093	CA	ARG	A	288		2.769	5.969	15.083	1.00	42.96
2094	C	ARG	A	288		3.269	5.379	13.774	1.00	42.65
2095	O	ARG	A	288		3.015	4.219	13.465	1.00	42.61
2096	CB	ARG	A	288		1.613	6.940	14.836	1.00	45.04
2097	CG	ARG	A	288		0.425	6.321	14.128	1.00	48.66
2098	CD	ARG	A	288		-0.811	7.210	14.128	1.00	51.29
2099	NE	ARG	A	288		-0.651	8.364	13.243	1.00	53.75
2100	CZ	ARG	A	288		-0.499	9.617	13.668	1.00	54.99

**FIG. 2-34A**





2121	CA	ILE	A	292	6.300	1.395	18.562	1.00	44.50
2122	C	ILE	A	292	5.816	2.343	19.650	1.00	45.65
2123	O	ILE	A	292	5.155	3.335	19.342	1.00	46.14
2124	CB	ILE	A	292	7.833	1.360	18.544	1.00	43.75
2125	CG1	ILE	A	292	8.408	2.772	18.452	1.00	43.53
2126	CG2	ILE	A	292	8.345	0.488	17.399	1.00	43.48
2127	CD1	ILE	A	292	9.919	2.823	18.411	1.00	43.81
2128	N	GLU	A	293	6.139	2.028	20.896	1.00	46.56
2129	CA	GLU	A	293	5.750	2.864	22.029	1.00	47.85
2130	C	GLU	A	293	6.937	3.673	22.527	1.00	47.03
2131	O	GLU	A	293	8.089	3.286	22.313	1.00	46.47
2132	CB	GLU	A	293	5.186	1.973	23.133	1.00	50.62
2133	CG	GLU	A	293	3.680	1.735	23.051	1.00	53.57
2134	CD	GLU	A	293	3.132	1.252	24.385	1.00	55.85
2135	OE1	GLU	A	293	3.663	0.235	24.895	1.00	56.88
2136	OE2	GLU	A	293	2.191	1.876	24.929	1.00	56.96
2137	N	ALA	A	294	6.708	4.773	23.233	1.00	46.80
2138	CA	ALA	A	294	7.797	5.618	23.718	1.00	47.26
2139	C	ALA	A	294	8.843	4.831	24.484	1.00	47.74
2140	O	ALA	A	294	10.056	5.007	24.289	1.00	48.22
2141	CB	ALA	A	294	7.260	6.780	24.546	1.00	46.78
2142	N	SER	A	295	8.436	3.892	25.316	1.00	48.05

**FIG. 2-34C**

2143	CA	SER	A	295	9.257	3.037	26.133	1.00	47.63
2144	C	SER	A	295	10.346	2.265	25.410	1.00	46.97
2145	O	SER	A	295	11.303	1.793	26.057	1.00	47.56
2146	CB	SER	A	295	8.340	2.003	26.837	1.00	48.01
2147	OG	SER	A	295	8.027	0.966	25.905	1.00	48.28
2148	N	GLN	A	296	10.256	2.092	24.102	1.00	45.19
2149	CA	GLN	A	296	11.275	1.355	23.359	1.00	44.36
2150	C	GLN	A	296	12.408	2.264	22.917	1.00	42.95
2151	O	GLN	A	296	13.471	1.798	22.505	1.00	42.77
2152	CB	GLN	A	296	10.617	0.635	22.180	1.00	45.62
2153	CG	GLN	A	296	9.237	0.075	22.532	1.00	46.57
2154	CD	GLN	A	296	8.730	-0.897	21.494	1.00	47.79
2155	OE1	GLN	A	296	7.551	-0.881	21.125	1.00	48.74
2156	NE2	GLN	A	296	9.609	-1.763	21.001	1.00	48.30
2157	N	ILE	A	297	12.205	3.573	23.038	1.00	41.44
2158	CA	ILE	A	297	13.219	4.559	22.695	1.00	39.95
2159	C	ILE	A	297	14.281	4.624	23.787	1.00	38.41
2160	O	ILE	A	297	14.009	4.967	24.934	1.00	37.64
2161	CB	ILE	A	297	12.625	5.963	22.469	1.00	40.09
2162	CG1	ILE	A	297	11.659	5.978	21.279	1.00	39.62
2163	CG2	ILE	A	297	13.728	6.994	22.250	1.00	39.76
2164	CD1	ILE	A	297	12.247	5.455	19.990	1.00	39.49

**FIG. 2-35A**

2165	N	GLY	A	298	15.515	4.307	23.421	1.00	37.84
2166	CA	GLY	A	298	16.599	4.327	24.404	1.00	37.21
2167	C	GLY	A	298	17.183	5.719	24.557	1.00	37.35
2168	O	GLY	A	298	17.381	6.216	25.665	1.00	37.77
2169	N	TYR	A	299	17.447	6.354	23.420	1.00	37.03
2170	CA	TYR	A	299	18.092	7.654	23.391	1.00	35.98
2171	C	TYR	A	299	17.388	8.622	22.447	1.00	35.82
2172	O	TYR	A	299	17.030	8.314	21.312	1.00	35.55
2173	CB	TYR	A	299	19.551	7.463	22.983	1.00	36.16
2174	CG	TYR	A	299	20.319	8.708	22.633	1.00	36.96
2175	CD1	TYR	A	299	20.929	8.828	21.390	1.00	37.22
2176	CD2	TYR	A	299	20.456	9.757	23.535	1.00	37.10
2177	CE1	TYR	A	299	21.648	9.957	21.048	1.00	37.84
2178	CE2	TYR	A	299	21.165	10.893	23.204	1.00	37.79
2179	CZ	TYR	A	299	21.770	10.981	21.966	1.00	38.60
2180	OH	TYR	A	299	22.504	12.096	21.627	1.00	39.51
2181	N	VAL	A	300	17.222	9.841	22.938	1.00	34.63
2182	CA	VAL	A	300	16.664	10.948	22.185	1.00	33.18
2183	C	VAL	A	300	17.784	11.965	21.929	1.00	32.63

**FIG. 2-35B**



2206	CG	HIS	A	303	15.963	21.570	18.080	1.00	29.65
2207	ND1	HIS	A	303	16.740	21.478	16.942	1.00	30.47
2208	CD2	HIS	A	303	15.552	22.850	18.160	1.00	29.32
2209	CE1	HIS	A	303	16.792	22.660	16.355	1.00	30.67
2210	NE2	HIS	A	303	16.084	23.516	17.084	1.00	30.18
2211	N	GLY	A	304	17.545	20.716	21.499	1.00	30.19
2212	CA	GLY	A	304	18.260	21.378	22.551	1.00	31.04
2213	C	GLY	A	304	19.387	22.299	22.113	1.00	30.87
2214	O	GLY	A	304	20.568	21.962	22.172	1.00	30.26
2215	N	THR	A	305	19.016	23.502	21.704	1.00	30.59
2216	CA	THR	A	305	19.924	24.486	21.163	1.00	30.95
2217	C	THR	A	305	20.526	25.444	22.160	1.00	30.62
2218	O	THR	A	305	21.218	26.374	21.730	1.00	31.05
2219	CB	THR	A	305	19.167	25.300	20.073	1.00	31.44
2220	OG1	THR	A	305	18.143	26.079	20.709	1.00	32.41
2221	CG2	THR	A	305	18.511	24.357	19.074	1.00	30.77
2222	N	SER	A	306	20.310	25.280	23.448	1.00	30.65
2223	CA	SER	A	306	20.823	26.156	24.492	1.00	29.52
2224	C	SER	A	306	20.129	27.510	24.521	1.00	29.40
2225	O	SER	A	306	20.713	28.556	24.800	1.00	28.21
2226	CB	SER	A	306	22.333	26.315	24.382	1.00	29.55
2227	OG	SER	A	306	22.887	26.873	25.564	1.00	29.38

**FIG. 2-36A**

2228	N	THR	A	307	18.828	27.513	24.218	1.00	30.00
2229	CA	THR	A	307	18.054	28.750	24.287	1.00	30.62
2230	C	THR	A	307	17.049	28.601	25.429	1.00	31.06
2231	O	THR	A	307	16.500	27.519	25.623	1.00	30.43
2232	CB	THR	A	307	17.330	29.115	22.986	1.00	29.95
2233	OG1	THR	A	307	16.320	28.137	22.714	1.00	29.62
2234	CG2	THR	A	307	18.318	29.199	21.834	1.00	29.18
2235	N	PRO	A	308	16.948	29.632	26.249	1.00	32.42
2236	CA	PRO	A	308	16.079	29.618	27.413	1.00	33.00
2237	C	PRO	A	308	14.725	29.019	27.109	1.00	34.60
2238	O	PRO	A	308	14.429	27.899	27.560	1.00	36.16
2239	CB	PRO	A	308	15.998	31.083	27.808	1.00	32.75
2240	CG	PRO	A	308	17.304	31.659	27.359	1.00	32.45
2241	CD	PRO	A	308	17.600	30.954	26.056	1.00	32.33
2242	N	ALA	A	309	13.936	29.674	26.262	1.00	35.22
2243	CA	ALA	A	309	12.602	29.191	25.929	1.00	35.74
2244	C	ALA	A	309	12.598	27.867	25.185	1.00	35.62
2245	O	ALA	A	309	11.768	26.998	25.490	1.00	36.25

**FIG. 2-36B**

[illegible]

**FIG. 2-36C**



2269	CA	ALA	A	313	9.625	23.450	25.595	1.00	38.76
2270	C	ALA	A	313	9.893	22.012	25.216	1.00	39.23
2271	O	ALA	A	313	9.032	21.158	25.441	1.00	40.34
2272	CB	ALA	A	313	9.401	24.290	24.340	1.00	38.69
2273	N	GLU	A	314	11.061	21.713	24.651	1.00	39.89
2274	CA	GLU	A	314	11.354	20.344	24.246	1.00	40.45
2275	C	GLU	A	314	11.322	19.373	25.418	1.00	40.84
2276	O	GLU	A	314	10.768	18.279	25.320	1.00	40.97
2277	CB	GLU	A	314	12.721	20.240	23.564	1.00	40.99
2278	CG	GLU	A	314	12.961	18.830	23.011	1.00	40.54
2279	CD	GLU	A	314	14.188	18.798	22.132	1.00	40.81
2280	OE1	GLU	A	314	14.953	19.783	22.149	1.00	40.94
2281	OE2	GLU	A	314	14.361	17.791	21.423	1.00	41.62
2282	N	ALA	A	315	11.963	19.767	26.514	1.00	41.04
2283	CA	ALA	A	315	11.937	18.989	27.740	1.00	41.54
2284	C	ALA	A	315	10.495	18.632	28.093	1.00	41.87
2285	O	ALA	A	315	10.175	17.464	28.313	1.00	41.76
2286	CB	ALA	A	315	12.588	19.759	28.877	1.00	41.38
2287	N	GLN	A	316	9.621	19.640	28.103	1.00	42.34
2288	CA	GLN	A	316	8.217	19.395	28.399	1.00	43.86
2289	C	GLN	A	316	7.595	18.404	27.423	1.00	44.27

**FIG. 2-37A**

2290	O	GLN	A	316	6.988	17.400	27.803	1.00	43.96
2291	CB	GLN	A	316	7.412	20.695	28.386	1.00	44.58
2292	CG	GLN	A	316	5.971	20.493	28.849	1.00	46.52
2293	CD	GLN	A	316	5.893	20.074	30.312	1.00	47.74
2294	OE1	GLN	A	316	6.524	20.669	31.190	1.00	47.58
2295	NE2	GLN	A	316	5.130	19.006	30.546	1.00	47.69
2296	N	ALA	A	317	7.864	18.596	26.130	1.00	44.25
2297	CA	ALA	A	317	7.349	17.688	25.118	1.00	44.89
2298	C	ALA	A	317	7.812	16.258	25.346	1.00	44.92
2299	O	ALA	A	317	7.103	15.311	24.979	1.00	44.45
2300	CB	ALA	A	317	7.760	18.188	23.734	1.00	45.79
2301	N	VAL	A	318	9.008	16.071	25.897	1.00	45.09
2302	CA	VAL	A	318	9.525	14.735	26.187	1.00	45.96
2303	C	VAL	A	318	8.773	14.126	27.372	1.00	46.69
2304	O	VAL	A	318	8.442	12.943	27.383	1.00	46.39
2305	CB	VAL	A	318	11.038	14.753	26.459	1.00	45.52
2306	CG1	VAL	A	318	11.526	13.458	27.096	1.00	45.04
2307	CG2	VAL	A	318	11.806	15.009	25.166	1.00	44.92
2308	N	LYS	A	319	8.439	14.958	28.352	1.00	47.66
2309	CA	LYS	A	319	7.685	14.521	29.517	1.00	49.06
2310	C	LYS	A	319	6.271	14.119	29.128	1.00	49.78

**FIG. 2-37B**

2311	O	LYS	A	319	5.722	13.163	29.680	1.00	50.92
2312	CB	LYS	A	319	7.689	15.604	30.598	1.00	49.56
2313	CG	LYS	A	319	9.083	15.838	31.176	1.00	50.90
2314	CD	LYS	A	319	9.067	16.783	32.366	1.00	52.01
2315	CE	LYS	A	319	9.207	16.011	33.668	1.00	53.29
2316	NZ	LYS	A	319	9.356	16.912	34.850	1.00	53.92
2317	N	THR	A	320	5.698	14.790	28.141	1.00	49.61
2318	CA	THR	A	320	4.377	14.478	27.627	1.00	49.41
2319	C	THR	A	320	4.383	13.153	26.878	1.00	50.24
2320	O	THR	A	320	3.445	12.365	27.009	1.00	51.00
2321	CB	THR	A	320	3.874	15.591	26.688	1.00	48.97
2322	OG1	THR	A	320	3.544	16.754	27.464	1.00	48.43
2323	CG2	THR	A	320	2.655	15.160	25.895	1.00	48.62
2324	N	ILE	A	321	5.396	12.928	26.060	1.00	51.08
2325	CA	ILE	A	321	5.482	11.731	25.236	1.00	52.44
2326	C	ILE	A	321	5.988	10.521	25.994	1.00	53.78
2327	O	ILE	A	321	5.453	9.413	25.850	1.00	54.21
2328	CB	ILE	A	321	6.389	11.992	24.012	1.00	52.16
2329	CG1	ILE	A	321	5.814	13.143	23.185	1.00	52.52
2330	CG2	ILE	A	321	6.559	10.745	23.168	1.00	51.63
2331	CD1	ILE	A	321	4.434	12.868	22.619	1.00	53.06

**FIG. 2-37C**

2332	N	PHE	A	322	7.062	10.686	26.764	1.00	55.32
2333	CA	PHE	A	322	7.623	9.536	27.482	1.00	57.01
2334	C	PHE	A	322	6.854	9.233	28.751	1.00	58.22
2335	O	PHE	A	322	6.709	8.063	29.131	1.00	58.09
2336	CB	PHE	A	322	9.129	9.740	27.695	1.00	56.37
2337	CG	PHE	A	322	9.837	9.510	26.375	1.00	56.26
2338	CD1	PHE	A	322	9.909	10.521	25.438	1.00	56.23
2339	CD2	PHE	A	322	10.364	8.269	26.073	1.00	56.06
2340	CE1	PHE	A	322	10.527	10.306	24.219	1.00	56.27
2341	CE2	PHE	A	322	10.981	8.052	24.857	1.00	56.46
2342	CZ	PHE	A	322	11.063	9.069	23.926	1.00	56.24
2343	N	GLY	A	323	6.262	10.257	29.358	1.00	59.40
2344	CA	GLY	A	323	5.449	10.098	30.548	1.00	61.56
2345	C	GLY	A	323	6.205	9.479	31.715	1.00	63.08
2346	O	GLY	A	323	7.035	10.135	32.346	1.00	62.72
2347	N	GLU	A	324	5.911	8.211	31.997	1.00	64.65
2348	CA	GLU	A	324	6.532	7.504	33.112	1.00	66.18
2349	C	GLU	A	324	7.932	7.025	32.757	1.00	65.94
2350	O	GLU	A	324	8.799	6.936	33.631	1.00	66.15
2351	CB	GLU	A	324	5.653	6.337	33.561	1.00	67.61
2352	CG	GLU	A	324	4.724	6.673	34.715	1.00	69.11
2353	CD	GLU	A	324	3.266	6.766	34.309	1.00	70.22

**FIG. 2-38A**

2354	OE1	GLU	A	324	2.919	7.668	33.508	1.00	70.44
2355	OE2	GLU	A	324	2.459	5.940	34.799	1.00	70.43
2356	N	ALA	A	325	8.170	6.761	31.475	1.00	65.16
2357	CA	ALA	A	325	9.469	6.309	31.002	1.00	64.72
2358	C	ALA	A	325	10.416	7.477	30.754	1.00	64.29
2359	O	ALA	A	325	11.565	7.276	30.360	1.00	63.88
2360	CB	ALA	A	325	9.326	5.470	29.739	1.00	64.73
2361	N	ALA	A	326	9.977	8.690	31.052	1.00	63.99
2362	CA	ALA	A	326	10.745	9.905	30.917	1.00	63.96
2363	C	ALA	A	326	12.013	9.906	31.759	1.00	64.59
2364	O	ALA	A	326	12.982	10.590	31.423	1.00	65.46
2365	CB	ALA	A	326	9.892	11.111	31.296	1.00	63.23
2366	N	SER	A	327	12.034	9.169	32.856	1.00	64.91
2367	CA	SER	A	327	13.195	9.076	33.724	1.00	64.87
2368	C	SER	A	327	14.168	8.006	33.253	1.00	64.31
2369	O	SER	A	327	15.363	8.062	33.553	1.00	65.08
2370	CB	SER	A	327	12.725	8.745	35.152	1.00	65.49
2371	OG	SER	A	327	11.692	7.767	35.086	1.00	65.92
2372	N	ARG	A	328	13.663	7.014	32.526	1.00	63.15

**FIG. 2-38B**

2373	CA	ARG	A	328	14.520	5.936	32.040	1.00	61.76
2374	C	ARG	A	328	15.101	6.250	30.671	1.00	59.76
2375	O	ARG	A	328	16.033	5.564	30.233	1.00	60.32
2376	CB	ARG	A	328	13.764	4.609	32.025	1.00	62.86
2377	CG	ARG	A	328	12.866	4.373	30.827	1.00	64.26
2378	CD	ARG	A	328	11.855	3.269	31.095	1.00	65.68
2379	NE	ARG	A	328	11.950	2.167	30.144	1.00	66.47
2380	CZ	ARG	A	328	11.064	1.187	30.020	1.00	66.85
2381	NH1	ARG	A	328	9.983	1.158	30.792	1.00	67.11
2382	NH2	ARG	A	328	11.246	0.229	29.119	1.00	67.06
2383	N	VAL	A	329	14.570	7.262	29.985	1.00	56.58
2384	CA	VAL	A	329	15.070	7.594	28.651	1.00	52.91
2385	C	VAL	A	329	16.235	8.569	28.713	1.00	51.13
2386	O	VAL	A	329	16.259	9.466	29.550	1.00	50.77
2387	CB	VAL	A	329	13.964	8.144	27.740	1.00	52.48
2388	CG1	VAL	A	329	13.541	9.544	28.160	1.00	51.82
2389	CG2	VAL	A	329	14.411	8.119	26.284	1.00	51.86
2390	N	LEU	A	330	17.217	8.350	27.844	1.00	48.78
2391	CA	LEU	A	330	18.386	9.205	27.748	1.00	46.67
2392	C	LEU	A	330	18.182	10.298	26.701	1.00	45.85
2393	O	LEU	A	330	17.791	10.038	25.560	1.00	45.82
2394	CB	LEU	A	330	19.627	8.379	27.404	1.00	46.55

**FIG. 2-38C**

2395	CG	LEU	A	330	20.032	7.297	28.410	1.00	46.63
2396	CD1	LEU	A	330	21.221	6.501	27.896	1.00	46.07
2397	CD2	LEU	A	330	20.345	7.902	29.769	1.00	45.97
2398	N	VAL	A	331	18.358	11.547	27.118	1.00	43.84
2399	CA	VAL	A	331	18.211	12.702	26.266	1.00	42.46
2400	C	VAL	A	331	19.460	13.580	26.316	1.00	41.99
2401	O	VAL	A	331	19.603	14.358	27.267	1.00	41.78
2402	CB	VAL	A	331	17.022	13.610	26.674	1.00	42.13
2403	CG1	VAL	A	331	16.686	14.548	25.519	1.00	41.88
2404	CG2	VAL	A	331	15.797	12.845	27.111	1.00	41.37
2405	N	SER	A	332	20.281	13.610	25.269	1.00	41.05
2406	CA	SER	A	332	21.423	14.534	25.294	1.00	39.11
2407	C	SER	A	332	21.364	15.492	24.113	1.00	38.45
2408	O	SER	A	332	20.643	15.253	23.151	1.00	38.77
2409	CB	SER	A	332	22.754	13.797	25.309	1.00	38.87
2410	OG	SER	A	332	22.976	13.032	24.140	1.00	38.04
2411	N	SER	A	333	22.152	16.557	24.185	1.00	37.37
2412	CA	SER	A	333	22.327	17.480	23.081	1.00	35.80
2413	C	SER	A	333	23.808	17.578	22.713	1.00	35.02
2414	O	SER	A	333	24.608	18.160	23.448	1.00	34.17
2415	CB	SER	A	333	21.803	18.883	23.391	1.00	35.80
2416	OG	SER	A	333	22.173	19.787	22.353	1.00	34.77

**FIG. 2-39A**

2417	N	THR	A	334	24.153	17.125	21.506	1.00	33.66
2418	CA	THR	A	334	25.523	17.226	21.031	1.00	32.68
2419	C	THR	A	334	25.890	18.626	20.566	1.00	31.79
2420	O	THR	A	334	27.042	18.855	20.175	1.00	32.24
2421	CB	THR	A	334	25.794	16.248	19.874	1.00	33.55
2422	OG1	THR	A	334	24.632	16.210	19.035	1.00	35.08
2423	CG2	THR	A	334	26.091	14.854	20.395	1.00	33.98
2424	N	LYS	A	335	24.966	19.571	20.620	1.00	29.86
2425	CA	LYS	A	335	25.130	20.954	20.255	1.00	28.11
2426	C	LYS	A	335	25.909	21.722	21.323	1.00	28.33
2427	O	LYS	A	335	26.403	22.833	21.112	1.00	28.49
2428	CB	LYS	A	335	23.766	21.632	20.065	1.00	27.41
2429	CG	LYS	A	335	22.985	21.211	18.848	1.00	26.22
2430	CD	LYS	A	335	21.797	22.117	18.573	1.00	25.45
2431	CE	LYS	A	335	21.096	21.719	17.274	1.00	24.18
2432	NZ	LYS	A	335	20.513	20.357	17.370	1.00	22.35
2433	N	SER	A	336	26.063	21.085	22.485	1.00	27.13
2434	CA	SER	A	336	26.898	21.586	23.553	1.00	26.20

**FIG. 2-39B**



2435	C	SER	A	336	28.357	21.641	23.098	1.00	25.15
2436	O	SER	A	336	29.092	22.541	23.491	1.00	24.26
2437	CB	SER	A	336	26.778	20.723	24.803	1.00	26.48
2438	OG	SER	A	336	26.951	19.355	24.499	1.00	26.89
2439	N	MET	A	337	28.738	20.692	22.253	1.00	24.47
2440	CA	MET	A	337	30.088	20.611	21.733	1.00	25.03
2441	C	MET	A	337	30.227	21.244	20.352	1.00	25.59
2442	O	MET	A	337	31.126	22.030	20.063	1.00	27.27
2443	CB	MET	A	337	30.505	19.123	21.646	1.00	23.76
2444	CG	MET	A	337	30.336	18.420	22.987	1.00	22.85
2445	SD	MET	A	337	30.647	16.670	22.961	1.00	22.05
2446	CE	MET	A	337	29.019	15.966	22.795	1.00	20.77
2447	N	THR	A	338	29.335	20.877	19.481	1.00	24.93
2448	CA	THR	A	338	29.336	21.064	18.043	1.00	24.13
2449	C	THR	A	338	28.770	22.406	17.637	1.00	24.84
2450	O	THR	A	338	29.244	23.073	16.706	1.00	25.40
2451	CB	THR	A	338	28.506	19.864	17.512	1.00	23.52
2452	OG1	THR	A	338	29.316	18.985	16.726	1.00	22.42
2453	CG2	THR	A	338	27.262	20.277	16.790	1.00	23.55
2454	N	GLY	A	339	27.753	22.870	18.368	1.00	24.13
2455	CA	GLY	A	339	27.098	24.144	18.051	1.00	21.84
2456	C	GLY	A	339	25.883	23.812	17.178	1.00	21.27
2457	O	GLY	A	339	25.688	22.635	16.865	1.00	21.79

**FIG. 2-39C**

2458	N	HIS	A	340	25.078	24.779	16.805	1.00	20.63
2459	CA	HIS	A	340	23.911	24.536	15.968	1.00	21.54
2460	C	HIS	A	340	24.257	24.569	14.493	1.00	21.15
2461	O	HIS	A	340	24.500	25.668	13.973	1.00	21.62
2462	CB	HIS	A	340	22.858	25.630	16.248	1.00	23.15
2463	CG	HIS	A	340	21.477	25.188	15.873	1.00	24.70
2464	ND1	HIS	A	340	21.254	24.220	14.915	1.00	25.46
2465	CD2	HIS	A	340	20.258	25.566	16.319	1.00	24.88
2466	CE1	HIS	A	340	19.955	24.014	14.797	1.00	25.60
2467	NE2	HIS	A	340	19.332	24.819	15.640	1.00	25.55
2468	N	LEU	A	341	24.136	23.463	13.765	1.00	21.78
2469	CA	LEU	A	341	24.425	23.446	12.332	1.00	21.51
2470	C	LEU	A	341	23.246	23.864	11.455	1.00	20.67
2471	O	LEU	A	341	23.264	23.596	10.245	1.00	20.80
2472	CB	LEU	A	341	24.939	22.111	11.840	1.00	22.08
2473	CG	LEU	A	341	26.253	21.519	12.279	1.00	23.06
2474	CD1	LEU	A	341	27.036	20.962	11.093	1.00	22.21
2475	CD2	LEU	A	341	27.124	22.487	13.058	1.00	23.72
2476	N	LEU	A	342	22.235	24.517	12.005	1.00	19.56
2477	CA	LEU	A	342	21.091	24.989	11.221	1.00	18.26
2478	C	LEU	A	342	20.559	23.973	10.240	1.00	18.01
2479	O	LEU	A	342	20.095	22.884	10.652	1.00	18.33

**FIG. 2-40A**

2480	CB	LEU	A	342	21.537	26.296	10.539	1.00	17.17
2481	CG	LEU	A	342	22.146	27.319	11.515	1.00	16.80
2482	CD1	LEU	A	342	22.711	28.519	10.799	1.00	16.76
2483	CD2	LEU	A	342	21.099	27.764	12.537	1.00	17.23
2484	N	GLY	A	343	20.749	24.167	8.940	1.00	16.41
2485	CA	GLY	A	343	20.241	23.256	7.937	1.00	15.90
2486	C	GLY	A	343	20.886	21.889	7.985	1.00	17.08
2487	O	GLY	A	343	20.296	20.916	7.502	1.00	18.05
2488	N	ALA	A	344	22.065	21.769	8.575	1.00	17.39
2489	CA	ALA	A	344	22.809	20.531	8.651	1.00	18.18
2490	C	ALA	A	344	22.583	19.807	9.966	1.00	19.20
2491	O	ALA	A	344	22.784	18.593	10.077	1.00	20.60
2492	CB	ALA	A	344	24.297	20.832	8.466	1.00	18.23
2493	N	ALA	A	345	22.134	20.542	10.974	1.00	19.41
2494	CA	ALA	A	345	21.900	19.977	12.300	1.00	19.17
2495	C	ALA	A	345	21.211	18.626	12.284	1.00	19.03
2496	O	ALA	A	345	21.746	17.655	12.825	1.00	19.54
2497	CB	ALA	A	345	21.118	20.990	13.127	1.00	19.37
2498	N	GLY	A	346	20.031	18.481	11.700	1.00	19.05
2499	CA	GLY	A	346	19.302	17.240	11.616	1.00	18.25
2500	C	GLY	A	346	20.038	16.124	10.895	1.00	18.83

**FIG. 2-40B**

2501	O	GLY	A	346	19.819	14.936	11.171	1.00	18.01
2502	N	ALA	A	347	20.907	16.443	9.944	1.00	19.83
2503	CA	ALA	A	347	21.683	15.439	9.228	1.00	21.04
2504	C	ALA	A	347	22.782	14.842	10.108	1.00	22.71
2505	O	ALA	A	347	22.859	13.614	10.275	1.00	23.84
2506	CB	ALA	A	347	22.311	16.035	7.979	1.00	19.88
2507	N	VAL	A	348	23.650	15.698	10.660	1.00	21.96
2508	CA	VAL	A	348	24.717	15.167	11.500	1.00	22.97
2509	C	VAL	A	348	24.116	14.420	12.684	1.00	24.48
2510	O	VAL	A	348	24.481	13.283	12.973	1.00	24.55
2511	CB	VAL	A	348	25.723	16.226	11.966	1.00	22.43
2512	CG1	VAL	A	348	26.341	16.954	10.786	1.00	20.44
2513	CG2	VAL	A	348	25.108	17.219	12.947	1.00	22.09
2514	N	GLU	A	349	23.120	14.982	13.349	1.00	26.69
2515	CA	GLU	A	349	22.474	14.348	14.490	1.00	29.09
2516	C	GLU	A	349	21.792	13.035	14.192	1.00	29.44
2517	O	GLU	A	349	21.603	12.239	15.125	1.00	29.84
2518	CB	GLU	A	349	21.503	15.364	15.131	1.00	30.54
2519	CG	GLU	A	349	22.309	16.556	15.629	1.00	33.46
2520	CD	GLU	A	349	21.540	17.774	16.041	1.00	35.00

**FIG. 2-40C**

2521	OE1	GLU	A	349	20.333	17.684	16.369	1.00	36.57
2522	OE2	GLU	A	349	22.176	18.863	16.064	1.00	35.08
2523	N	SER	A	350	21.411	12.764	12.952	1.00	29.09
2524	CA	SER	A	350	20.905	11.481	12.516	1.00	28.77
2525	C	SER	A	350	22.049	10.458	12.529	1.00	29.04
2526	O	SER	A	350	21.839	9.297	12.841	1.00	29.05
2527	CB	SER	A	350	20.348	11.539	11.089	1.00	28.76
2528	OG	SER	A	350	19.043	12.076	11.069	1.00	28.97
2529	N	ILE	A	351	23.246	10.918	12.176	1.00	28.95
2530	CA	ILE	A	351	24.426	10.066	12.186	1.00	29.01
2531	C	ILE	A	351	24.801	9.724	13.627	1.00	29.32
2532	O	ILE	A	351	25.060	8.551	13.918	1.00	29.82
2533	CB	ILE	A	351	25.611	10.703	11.453	1.00	28.57
2534	CG1	ILE	A	351	25.423	10.556	9.941	1.00	28.77
2535	CG2	ILE	A	351	26.940	10.091	11.861	1.00	28.44
2536	CD1	ILE	A	351	26.265	11.488	9.099	1.00	28.88
2537	N	TYR	A	352	24.714	10.695	14.530	1.00	28.96
2538	CA	TYR	A	352	25.000	10.452	15.938	1.00	29.99
2539	C	TYR	A	352	24.004	9.479	16.562	1.00	30.75
2540	O	TYR	A	352	24.407	8.671	17.391	1.00	32.84
2541	CB	TYR	A	352	25.012	11.723	16.779	1.00	28.66

**FIG. 2-41A**

2542	CG	TYR	A	352				25.850	12.864	16.269	1.00	26.47
2543	CD1	TYR	A	352				25.545	14.168	16.639	1.00	26.55
2544	CD2	TYR	A	352				26.948	12.650	15.451	1.00	25.98
2545	CE1	TYR	A	352				26.313	15.236	16.196	1.00	26.27
2546	CE2	TYR	A	352				27.708	13.705	14.984	1.00	26.13
2547	CZ	TYR	A	352				27.385	14.991	15.359	1.00	25.70
2548	OH	TYR	A	352				28.157	16.019	14.896	1.00	25.41
2549	N	SER	A	353				22.744	9.528	16.167	1.00	31.38
2550	CA	SER	A	353				21.742	8.592	16.666	1.00	32.24
2551	C	SER	A	353				21.926	7.201	16.064	1.00	32.63
2552	O	SER	A	353				21.565	6.189	16.681	1.00	32.93
2553	CB	SER	A	353				20.337	9.125	16.385	1.00	32.06
2554	OG	SER	A	353				20.266	10.510	16.706	1.00	32.40
2555	N	ILE	A	354				22.497	7.136	14.866	1.00	31.79
2556	CA	ILE	A	354				22.761	5.860	14.218	1.00	31.51
2557	C	ILE	A	354				23.987	5.200	14.844	1.00	32.97
2558	O	ILE	A	354				23.951	4.012	15.168	1.00	33.27
2559	CB	ILE	A	354				22.935	6.018	12.703	1.00	29.87
2560	CG1	ILE	A	354				21.576	6.159	12.009	1.00	29.52

**FIG. 2-41B**

2561	CG2	ILE	A	354	23.698	4.848	12.116	1.00	30.35
2562	CD1	ILE	A	354	21.606	6.908	10.688	1.00	27.41
2563	N	LEU	A	355	25.055	5.970	15.066	1.00	33.53
2564	CA	LEU	A	355	26.290	5.432	15.639	1.00	33.26
2565	C	LEU	A	355	26.082	4.959	17.072	1.00	33.69
2566	O	LEU	A	355	26.622	3.935	17.510	1.00	32.84
2567	CB	LEU	A	355	27.439	6.436	15.553	1.00	32.20
2568	CG	LEU	A	355	27.931	6.753	14.130	1.00	31.40
2569	CD1	LEU	A	355	28.833	7.978	14.145	1.00	31.15
2570	CD2	LEU	A	355	28.643	5.566	13.506	1.00	29.67
2571	N	ALA	A	356	25.232	5.673	17.809	1.00	33.95
2572	CA	ALA	A	356	24.883	5.298	19.175	1.00	34.20
2573	C	ALA	A	356	24.327	3.879	19.202	1.00	35.31
2574	O	ALA	A	356	24.632	3.095	20.103	1.00	35.75
2575	CB	ALA	A	356	23.883	6.300	19.720	1.00	33.94
2576	N	LEU	A	357	23.556	3.497	18.178	1.00	36.14
2577	CA	LEU	A	357	23.049	2.136	18.063	1.00	36.56
2578	C	LEU	A	357	24.201	1.160	17.855	1.00	37.61
2579	O	LEU	A	357	24.258	0.103	18.490	1.00	39.13
2580	CB	LEU	A	357	22.020	2.012	16.933	1.00	35.23
2581	CG	LEU	A	357	20.692	2.753	17.197	1.00	34.83
2582	CD1	LEU	A	357	19.880	2.899	15.923	1.00	33.45
2583	CD2	LEU	A	357	19.892	2.060	18.281	1.00	33.22

**FIG. 2-41C**

2584	N	ARG	A	358	25.135	1.515	16.982	1.00	37.51
2585	CA	ARG	A	358	26.271	0.683	16.685	1.00	37.58
2586	C	ARG	A	358	27.129	0.376	17.910	1.00	38.26
2587	O	ARG	A	358	27.577	-0.751	18.097	1.00	39.24
2588	CB	ARG	A	358	27.197	1.380	15.656	1.00	37.33
2589	CG	ARG	A	358	28.337	0.451	15.242	1.00	37.76
2590	CD	ARG	A	358	29.272	1.085	14.228	1.00	37.44
2591	NE	ARG	A	358	30.034	2.160	14.848	1.00	38.18
2592	CZ	ARG	A	358	30.884	2.965	14.221	1.00	38.70
2593	NH1	ARG	A	358	31.108	2.831	12.917	1.00	38.32
2594	NH2	ARG	A	358	31.479	3.932	14.919	1.00	38.15
2595	N	ASP	A	359	27.448	1.410	18.670	1.00	37.94
2596	CA	ASP	A	359	28.406	1.368	19.746	1.00	37.27
2597	C	ASP	A	359	27.808	1.313	21.132	1.00	38.02
2598	O	ASP	A	359	28.521	1.217	22.136	1.00	37.65
2599	CB	ASP	A	359	29.231	2.675	19.670	1.00	36.75
2600	CG	ASP	A	359	30.238	2.668	18.549	1.00	36.38
2601	OD1	ASP	A	359	30.280	1.693	17.771	1.00	36.72
2602	OD2	ASP	A	359	30.991	3.661	18.460	1.00	36.33
2603	N	GLN	A	360	26.491	1.483	21.216	1.00	38.96
2604	CA	GLN	A	360	25.810	1.516	22.509	1.00	39.05

**FIG. 2-42A**



2605	C	GLN	A	360	26.538	2.465	23.461	1.00	39.38
2606	O	GLN	A	360	26.698	2.168	24.643	1.00	39.53
2607	CB	GLN	A	360	25.660	0.130	23.099	1.00	39.41
2608	CG	GLN	A	360	24.973	-0.898	22.217	1.00	39.76
2609	CD	GLN	A	360	23.466	-0.769	22.178	1.00	40.29
2610	OE1	GLN	A	360	22.782	-0.477	23.159	1.00	39.32
2611	NE2	GLN	A	360	22.893	-0.991	20.988	1.00	40.99
2612	N	ALA	A	361	26.886	3.644	22.959	1.00	39.00
2613	CA	ALA	A	361	27.461	4.728	23.751	1.00	38.72
2614	C	ALA	A	361	26.683	6.012	23.442	1.00	38.04
2615	O	ALA	A	361	26.357	6.270	22.275	1.00	38.26
2616	CB	ALA	A	361	28.937	4.883	23.455	1.00	38.95
2617	N	VAL	A	362	26.325	6.779	24.460	1.00	35.95
2618	CA	VAL	A	362	25.509	7.982	24.250	1.00	33.68
2619	C	VAL	A	362	26.293	9.242	24.568	1.00	32.65
2620	O	VAL	A	362	26.684	9.490	25.703	1.00	31.11
2621	CB	VAL	A	362	24.215	7.874	25.077	1.00	33.18
2622	CG1	VAL	A	362	23.575	9.209	25.387	1.00	33.96
2623	CG2	VAL	A	362	23.209	6.988	24.346	1.00	32.67
2624	N	PRO	A	363	26.535	10.050	23.534	1.00	32.66
2625	CA	PRO	A	363	27.283	11.285	23.645	1.00	31.67

**FIG. 2-42B**

2626	C	PRO	A	363		26.671	12.173	24.705	1.00	31.09
2627	O	PRO	A	363		25.449	12.194	24.869	1.00	32.64
2628	CB	PRO	A	363		27.199	11.941	22.285	1.00	32.07
2629	CG	PRO	A	363		26.641	10.940	21.360	1.00	32.96
2630	CD	PRO	A	363		26.096	9.789	22.139	1.00	32.89
2631	N	PRO	A	364		27.495	12.901	25.434	1.00	30.09
2632	CA	PRO	A	364		27.032	13.733	26.516	1.00	29.72
2633	C	PRO	A	364		26.553	15.120	26.123	1.00	29.59
2634	O	PRO	A	364		26.782	15.591	25.016	1.00	28.83
2635	CB	PRO	A	364		28.284	13.863	27.386	1.00	29.18
2636	CG	PRO	A	364		29.418	13.799	26.423	1.00	29.36
2637	CD	PRO	A	364		28.974	12.883	25.323	1.00	29.95
2638	N	THR	A	365		25.950	15.787	27.100	1.00	28.90
2639	CA	THR	A	365		25.536	17.166	27.039	1.00	29.34
2640	C	THR	A	365		26.515	17.969	27.909	1.00	29.33
2641	O	THR	A	365		26.271	18.122	29.106	1.00	28.44
2642	CB	THR	A	365		24.119	17.418	27.589	1.00	30.33
2643	OG1	THR	A	365		23.174	16.540	26.967	1.00	31.73
2644	CG2	THR	A	365		23.680	18.864	27.360	1.00	29.24
2645	N	ILE	A	366		27.654	18.366	27.362	1.00	29.73
2646	CA	ILE	A	366		28.650	19.040	28.203	1.00	30.00

**FIG. 2-42C**

2647	C	ILE	A	366	28.162	20.419	28.621	1.00	31.27
2648	O	ILE	A	366	27.219	20.981	28.067	1.00	30.39
2649	CB	ILE	A	366	30.025	19.120	27.528	1.00	29.07
2650	CG1	ILE	A	366	30.052	20.205	26.451	1.00	29.20
2651	CG2	ILE	A	366	30.405	17.769	26.927	1.00	27.75
2652	CD1	ILE	A	366	31.415	20.552	25.913	1.00	28.17
2653	N	ASN	A	367	28.785	20.975	29.652	1.00	32.72
2654	CA	ASN	A	367	28.511	22.285	30.190	1.00	34.91
2655	C	ASN	A	367	27.251	22.403	31.019	1.00	36.61
2656	O	ASN	A	367	26.871	23.504	31.450	1.00	36.20
2657	CB	ASN	A	367	28.483	23.311	29.038	1.00	35.89
2658	CG	ASN	A	367	29.871	23.565	28.480	1.00	36.26
2659	OD1	ASN	A	367	30.866	23.259	29.146	1.00	37.27
2660	ND2	ASN	A	367	29.952	24.113	27.279	1.00	35.83
2661	N	LEU	A	368	26.596	21.297	31.326	1.00	39.08
2662	CA	LEU	A	368	25.351	21.292	32.094	1.00	41.70
2663	C	LEU	A	368	25.647	21.267	33.592	1.00	44.25
2664	O	LEU	A	368	25.388	20.294	34.299	1.00	44.89
2665	CB	LEU	A	368	24.506	20.106	31.655	1.00	40.63
2666	CG	LEU	A	368	23.160	19.841	32.309	1.00	40.11
2667	CD1	LEU	A	368	22.287	21.085	32.347	1.00	40.15

**FIG. 2-43A**

2668	CD2	LEU	A	368	22.447	18.702	31.590	1.00	38.98
2669	N	ASP	A	369	26.196	22.375	34.085	1.00	46.52
2670	CA	ASP	A	369	26.643	22.493	35.460	1.00	48.49
2671	C	ASP	A	369	25.472	22.540	36.426	1.00	49.89
2672	O	ASP	A	369	25.518	21.893	37.476	1.00	50.35
2673	CB	ASP	A	369	27.544	23.715	35.641	1.00	48.44
2674	CG	ASP	A	369	28.783	23.682	34.769	1.00	48.89
2675	OD1	ASP	A	369	29.283	24.771	34.401	1.00	49.53
2676	OD2	ASP	A	369	29.284	22.587	34.435	1.00	48.33
2677	N	ASN	A	370	24.430	23.299	36.104	1.00	51.52
2678	CA	ASN	A	370	23.261	23.423	36.964	1.00	52.70
2679	C	ASN	A	370	21.951	23.438	36.185	1.00	53.77
2680	O	ASN	A	370	21.512	24.515	35.756	1.00	53.47
2681	CB	ASN	A	370	23.326	24.734	37.759	1.00	52.88
2682	CG	ASN	A	370	24.420	24.856	38.775	1.00	53.02
2683	OD1	ASN	A	370	25.288	25.726	38.676	1.00	52.97
2684	ND2	ASN	A	370	24.419	23.967	39.766	1.00	53.88
2685	N	PRO	A	371	21.289	22.302	36.046	1.00	55.26
2686	CA	PRO	A	371	20.009	22.231	35.356	1.00	57.50
2687	C	PRO	A	371	19.056	23.295	35.870	1.00	60.20
2688	O	PRO	A	371	19.124	23.621	37.064	1.00	61.29

**FIG. 2-43B**

2689	CB	PRO	A	371	19.481	20.849	35.667	1.00	56.46
2690	CG	PRO	A	371	20.611	20.064	36.190	1.00	56.02
2691	CD	PRO	A	371	21.728	20.992	36.542	1.00	55.51
2692	N	ASP	A	372	18.181	23.849	35.029	1.00	63.07
2693	CA	ASP	A	372	17.273	24.869	35.590	1.00	66.12
2694	C	ASP	A	372	16.119	24.159	36.301	1.00	67.48
2695	O	ASP	A	372	15.977	22.938	36.253	1.00	67.01
2696	CB	ASP	A	372	16.848	25.919	34.606	1.00	66.67
2697	CG	ASP	A	372	16.102	25.455	33.384	1.00	67.57
2698	OD1	ASP	A	372	16.051	24.235	33.120	1.00	67.94
2699	OD2	ASP	A	372	15.548	26.313	32.657	1.00	67.93
2700	N	GLU	A	373	15.370	24.916	37.074	1.00	69.63
2701	CA	GLU	A	373	14.336	24.473	37.968	1.00	71.38
2702	C	GLU	A	373	13.674	23.139	37.710	1.00	71.44
2703	O	GLU	A	373	13.781	22.240	38.570	1.00	71.34
2704	CB	GLU	A	373	13.255	25.573	38.067	1.00	72.68
2705	CG	GLU	A	373	13.293	26.290	39.420	1.00	74.09
2706	CD	GLU	A	373	11.900	26.805	39.766	1.00	75.02
2707	OE1	GLU	A	373	11.719	28.038	39.754	1.00	75.05
2708	OE2	GLU	A	373	11.025	25.946	40.020	1.00	75.57
2709	N	GLY	A	374	12.842	23.002	36.683	1.00	71.36

**FIG. 2-43C**

2710	CA	GLY	A	374	12.019	21.821	36.531	1.00	71.79
2711	C	GLY	A	374	12.488	20.762	35.569	1.00	72.06
2712	O	GLY	A	374	11.663	19.944	35.116	1.00	72.74
2713	N	CYS	A	375	13.776	20.705	35.244	1.00	71.14
2714	CA	CYS	A	375	14.273	19.700	34.302	1.00	70.11
2715	C	CYS	A	375	14.845	18.495	35.029	1.00	69.27
2716	O	CYS	A	375	16.026	18.445	35.367	1.00	69.95
2717	CB	CYS	A	375	15.295	20.356	33.373	1.00	70.22
2718	SG	CYS	A	375	14.615	21.786	32.484	1.00	70.33
2719	N	ASP	A	376	14.003	17.492	35.257	1.00	67.38
2720	CA	ASP	A	376	14.353	16.293	35.989	1.00	65.40
2721	C	ASP	A	376	14.761	15.117	35.118	1.00	63.43
2722	O	ASP	A	376	14.848	13.977	35.602	1.00	63.21
2723	CB	ASP	A	376	13.144	15.872	36.851	1.00	66.52
2724	CG	ASP	A	376	11.940	15.452	36.031	1.00	67.35
2725	OD1	ASP	A	376	11.974	15.549	34.786	1.00	67.44
2726	OD2	ASP	A	376	10.925	15.017	36.628	1.00	67.75
2727	N	LEU	A	377	14.953	15.337	33.820	1.00	60.30
2728	CA	LEU	A	377	15.263	14.233	32.913	1.00	56.65
2729	C	LEU	A	377	16.745	13.893	32.912	1.00	54.35
2730	O	LEU	A	377	17.586	14.727	33.248	1.00	54.22
2731	CB	LEU	A	377	14.804	14.587	31.496	1.00	56.05

**FIG. 2-44A**

2732	CG	LEU	A	377	13.342	14.988	31.318	1.00	55.48
2733	CD1	LEU	A	377	13.151	15.780	30.034	1.00	55.31
2734	CD2	LEU	A	377	12.450	13.755	31.324	1.00	55.45
2735	N	ASP	A	378	17.072	12.669	32.518	1.00	51.50
2736	CA	ASP	A	378	18.466	12.246	32.405	1.00	49.45
2737	C	ASP	A	378	19.063	12.822	31.118	1.00	47.99
2738	O	ASP	A	378	18.941	12.271	30.023	1.00	47.05
2739	CB	ASP	A	378	18.579	10.724	32.418	1.00	49.34
2740	CG	ASP	A	378	19.988	10.196	32.572	1.00	48.74
2741	OD1	ASP	A	378	20.188	8.963	32.538	1.00	48.13
2742	OD2	ASP	A	378	20.931	11.003	32.733	1.00	49.41
2743	N	PHE	A	379	19.757	13.945	31.255	1.00	46.19
2744	CA	PHE	A	379	20.293	14.689	30.135	1.00	44.78
2745	C	PHE	A	379	21.708	14.267	29.762	1.00	44.38
2746	O	PHE	A	379	22.392	14.967	29.015	1.00	44.31
2747	CB	PHE	A	379	20.289	16.185	30.455	1.00	44.27
2748	CG	PHE	A	379	18.959	16.872	30.410	1.00	43.99
2749	CD1	PHE	A	379	18.592	17.747	31.419	1.00	43.84
2750	CD2	PHE	A	379	18.069	16.671	29.370	1.00	44.12
2751	CE1	PHE	A	379	17.374	18.397	31.397	1.00	43.77

**FIG. 2-44B**

2752	CE2	PHE	A	379	16.850	17.315	29.337	1.00	44.24
2753	CZ	PHE	A	379	16.497	18.184	30.358	1.00	43.96
2754	N	VAL	A	380	22.144	13.120	30.252	1.00	43.74
2755	CA	VAL	A	380	23.491	12.604	30.043	1.00	42.47
2756	C	VAL	A	380	24.485	13.738	30.306	1.00	42.16
2757	O	VAL	A	380	25.133	14.254	29.412	1.00	41.83
2758	CB	VAL	A	380	23.717	11.953	28.690	1.00	41.28
2759	CG1	VAL	A	380	25.002	11.135	28.721	1.00	40.26
2760	CG2	VAL	A	380	22.530	11.071	28.317	1.00	41.05
2761	N	PRO	A	381	24.545	14.148	31.578	1.00	42.27
2762	CA	PRO	A	381	25.180	15.367	31.990	1.00	42.11
2763	C	PRO	A	381	26.599	15.644	31.608	1.00	41.67
2764	O	PRO	A	381	26.806	16.781	31.118	1.00	43.27
2765	CB	PRO	A	381	25.021	15.391	33.511	1.00	42.44
2766	CG	PRO	A	381	23.830	14.555	33.781	1.00	42.72
2767	CD	PRO	A	381	23.743	13.541	32.680	1.00	42.38
2768	N	HIS	A	382	27.641	14.854	31.837	1.00	40.46
2769	CA	HIS	A	382	28.972	15.361	31.463	1.00	40.21
2770	C	HIS	A	382	29.808	14.418	30.635	1.00	41.00
2771	O	HIS	A	382	30.612	14.846	29.797	1.00	39.92
2772	CB	HIS	A	382	29.745	15.751	32.740	1.00	39.82

**FIG. 2-44C**



2773	CG	HIS	A	382	29.317	17.068	33.305	1.00	39.32
2774	ND1	HIS	A	382	29.629	18.266	32.705	1.00	39.09
2775	CD2	HIS	A	382	28.543	17.367	34.375	1.00	39.39
2776	CE1	HIS	A	382	29.086	19.250	33.393	1.00	39.48
2777	NE2	HIS	A	382	28.422	18.738	34.413	1.00	39.23
2778	N	GLU	A	383	29.706	13.118	30.916	1.00	42.14
2779	CA	GLU	A	383	30.521	12.126	30.227	1.00	43.32
2780	C	GLU	A	383	29.638	11.155	29.456	1.00	42.41
2781	O	GLU	A	383	28.503	10.903	29.847	1.00	41.73
2782	CB	GLU	A	383	31.403	11.362	31.220	1.00	45.87
2783	CG	GLU	A	383	32.071	12.198	32.299	1.00	48.56
2784	CD	GLU	A	383	33.412	12.759	31.859	1.00	50.99
2785	OE1	GLU	A	383	34.217	12.003	31.260	1.00	51.92
2786	OE2	GLU	A	383	33.672	13.962	32.105	1.00	52.07
2787	N	ALA	A	384	30.166	10.620	28.357	1.00	42.07
2788	CA	ALA	A	384	29.437	9.632	27.575	1.00	41.28
2789	C	ALA	A	384	28.935	8.511	28.488	1.00	41.42
2790	O	ALA	A	384	29.646	8.072	29.392	1.00	40.84
2791	CB	ALA	A	384	30.318	9.038	26.491	1.00	40.98
2792	N	ARG	A	385	27.719	8.050	28.221	1.00	41.17
2793	CA	ARG	A	385	27.134	6.969	28.987	1.00	41.16
2794	C	ARG	A	385	27.155	5.663	28.204	1.00	41.68

**FIG. 2-45A**

2795	O	ARG	A	385	26.740					27.048	1.00	43.05
2796	CB	ARG	A	385	25.688					29.379	1.00	41.25
2797	CG	ARG	A	385	25.008					30.128	1.00	41.15
2798	CD	ARG	A	385	24.890					31.606	1.00	40.96
2799	NE	ARG	A	385	23.866					31.831	1.00	41.21
2800	CZ	ARG	A	385	24.175					32.233	1.00	41.50
2801	NH1	ARG	A	385	25.455					32.428	1.00	41.34
2802	NH2	ARG	A	385	23.211					32.418	1.00	42.12
2803	N	GLN	A	386	27.568					28.867	1.00	41.57
2804	CA	GLN	A	386	27.548					28.264	1.00	40.47
2805	C	GLN	A	386	26.152					28.446	1.00	39.88
2806	O	GLN	A	386	25.497					29.451	1.00	39.50
2807	CB	GLN	A	386	28.622					28.935	1.00	41.01
2808	CG	GLN	A	386	28.533					28.674	1.00	40.91
2809	CD	GLN	A	386	29.158					27.341	1.00	41.24
2810	OE1	GLN	A	386	30.355					27.144	1.00	41.99
2811	NE2	GLN	A	386	28.338					26.430	1.00	41.97
2812	N	VAL	A	387	25.622					27.446	1.00	38.93

**FIG. 2-45B**

2813	CA	VAL	A	387	24.293	1.392	27.543	1.00	38.54
2814	C	VAL	A	387	24.315	-0.048	27.017	1.00	38.79
2815	O	VAL	A	387	25.250	-0.473	26.346	1.00	38.11
2816	CB	VAL	A	387	23.166	2.146	26.817	1.00	37.66
2817	CG1	VAL	A	387	22.938	3.547	27.358	1.00	36.33
2818	CG2	VAL	A	387	23.414	2.193	25.311	1.00	37.03
2819	N	SER	A	388	23.234	-0.770	27.273	1.00	39.59
2820	CA	SER	A	388	23.106	-2.146	26.786	1.00	40.66
2821	C	SER	A	388	21.701	-2.390	26.241	1.00	40.21
2822	O	SER	A	388	20.723	-1.842	26.761	1.00	40.50
2823	CB	SER	A	388	23.421	-3.127	27.922	1.00	41.01
2824	OG	SER	A	388	23.601	-4.451	27.431	1.00	41.76
2825	N	GLY	A	389	21.562	-3.180	25.192	1.00	39.76
2826	CA	GLY	A	389	20.284	-3.503	24.608	1.00	41.14
2827	C	GLY	A	389	19.426	-2.359	24.114	1.00	41.70
2828	O	GLY	A	389	18.189	-2.390	24.235	1.00	41.06
2829	N	MET	A	390	20.032	-1.330	23.533	1.00	42.05
2830	CA	MET	A	390	19.265	-0.199	23.001	1.00	42.20
2831	C	MET	A	390	18.906	-0.488	21.545	1.00	42.88
2832	O	MET	A	390	19.802	-0.610	20.705	1.00	42.82
2833	CB	MET	A	390	20.065	1.080	23.159	1.00	41.46
2834	CG	MET	A	390	19.354	2.345	22.696	1.00	40.33
2835	SD	MET	A	390	20.300	3.828	23.053	1.00	39.24

**FIG. 2-45C**

2836	CE	MET	A	390	21.765	3.567	22.063	1.00	37.25
2837	N	GLU	A	391	17.620	-0.654	21.248	1.00	43.99
2838	CA	GLU	A	391	17.201	-1.001	19.892	1.00	46.08
2839	C	GLU	A	391	16.864	0.206	19.024	1.00	45.41
2840	O	GLU	A	391	17.167	0.247	17.826	1.00	44.59
2841	CB	GLU	A	391	16.005	-1.963	19.929	1.00	48.01
2842	CG	GLU	A	391	16.255	-3.301	20.576	1.00	51.25
2843	CD	GLU	A	391	16.345	-4.482	19.632	1.00	53.60
2844	OE1	GLU	A	391	15.617	-4.540	18.607	1.00	54.36
2845	OE2	GLU	A	391	17.166	-5.391	19.930	1.00	54.27
2846	N	TYR	A	392	16.214	1.215	19.591	1.00	44.78
2847	CA	TYR	A	392	15.787	2.388	18.871	1.00	44.24
2848	C	TYR	A	392	16.312	3.695	19.477	1.00	43.65
2849	O	TYR	A	392	16.257	3.870	20.701	1.00	43.45
2850	CB	TYR	A	392	14.257	2.501	18.881	1.00	44.89
2851	CG	TYR	A	392	13.475	1.323	18.387	1.00	45.69
2852	CD1	TYR	A	392	12.942	0.403	19.287	1.00	46.27
2853	CD2	TYR	A	392	13.246	1.120	17.032	1.00	45.96
2854	CE1	TYR	A	392	12.202	-0.678	18.851	1.00	46.79
2855	CE2	TYR	A	392	12.515	0.037	16.588	1.00	46.86
2856	CZ	TYR	A	392	11.991	-0.857	17.499	1.00	47.26
2857	OH	TYR	A	392	11.240	-1.930	17.071	1.00	47.84
2858	N	THR	A	393	16.527	4.677	18.599	1.00	41.43

**FIG. 2-46A**

2859	CA	THR	A	393	16.763	6.049	18.998	1.00	40.27
2860	C	THR	A	393	15.896	7.031	18.195	1.00	39.59
2861	O	THR	A	393	15.601	6.863	17.017	1.00	39.19
2862	CB	THR	A	393	18.227	6.496	18.876	1.00	40.35
2863	OG1	THR	A	393	18.792	6.069	17.624	1.00	40.81
2864	CG2	THR	A	393	19.062	5.964	20.019	1.00	39.93
2865	N	LEU	A	394	15.488	8.104	18.846	1.00	39.00
2866	CA	LEU	A	394	14.695	9.169	18.264	1.00	38.29
2867	C	LEU	A	394	15.567	10.401	18.030	1.00	37.46
2868	O	LEU	A	394	16.480	10.682	18.814	1.00	36.71
2869	CB	LEU	A	394	13.533	9.523	19.189	1.00	39.52
2870	CG	LEU	A	394	12.508	10.542	18.696	1.00	40.53
2871	CD1	LEU	A	394	11.158	9.876	18.456	1.00	40.54
2872	CD2	LEU	A	394	12.360	11.689	19.690	1.00	40.98
2873	N	CYS	A	395	15.300	11.120	16.940	1.00	36.66
2874	CA	CYS	A	395	16.095	12.31 <sup>c</sup>	16.628	1.00	35.56
2875	C	CYS	A	395	15.238	13.530	16.318	1.00	34.76
2876	O	CYS	A	395	14.505	13.532	15.328	1.00	34.93

**FIG. 2-46B**

2877	CB	CYS	A	395	17.014	12.019	15.441	1.00	34.91
2878	SG	CYS	A	395	17.954	13.469	14.915	1.00	35.28
2879	N	ASN	A	396	15.362	14.594	17.099	1.00	33.67
2880	CA	ASN	A	396	14.583	15.799	16.915	1.00	33.78
2881	C	ASN	A	396	15.283	16.976	16.256	1.00	32.51
2882	O	ASN	A	396	16.488	17.152	16.339	1.00	33.78
2883	CB	ASN	A	396	14.115	16.318	18.292	1.00	35.61
2884	CG	ASN	A	396	12.854	15.629	18.754	1.00	37.03
2885	OD1	ASN	A	396	12.208	14.917	17.979	1.00	36.89
2886	ND2	ASN	A	396	12.542	15.844	20.031	1.00	37.90
2887	N	SER	A	397	14.501	17.847	15.645	1.00	31.24
2888	CA	SER	A	397	14.937	19.065	14.990	1.00	30.08
2889	C	SER	A	397	13.728	19.999	14.871	1.00	29.36
2890	O	SER	A	397	12.686	19.517	14.403	1.00	28.86
2891	CB	SER	A	397	15.460	18.847	13.579	1.00	29.66
2892	OG	SER	A	397	16.795	18.440	13.514	1.00	30.44
2893	N	PHE	A	398	13.798	21.220	15.377	1.00	28.10
2894	CA	PHE	A	398	12.630	22.116	15.262	1.00	28.51
2895	C	PHE	A	398	13.071	23.370	14.525	1.00	28.82
2896	O	PHE	A	398	14.295	23.555	14.417	1.00	30.86
2897	CB	PHE	A	398	12.006	22.417	16.613	1.00	28.54
2898	CG	PHE	A	398	11.817	21.230	17.522	1.00	28.25

**FIG. 2-46C**

2899	CD1	PHE	A	398	12.295	21.264	18.818	1.00	28.38
2900	CD2	PHE	A	398	11.174	20.084	17.096	1.00	27.71
2901	CE1	PHE	A	398	12.163	20.173	19.651	1.00	29.51
2902	CE2	PHE	A	398	11.073	18.976	17.897	1.00	28.62
2903	CZ	PHE	A	398	11.556	19.013	19.188	1.00	29.57
2904	N	GLY	A	399	12.192	24.182	13.950	1.00	27.59
2905	CA	GLY	A	399	12.635	25.341	13.198	1.00	26.19
2906	C	GLY	A	399	11.652	26.491	13.079	1.00	26.07
2907	O	GLY	A	399	10.445	26.378	13.285	1.00	25.91
2908	N	PHE	A	400	12.188	27.658	12.745	1.00	25.06
2909	CA	PHE	A	400	11.482	28.899	12.529	1.00	24.03
2910	C	PHE	A	400	10.259	28.629	11.651	1.00	24.31
2911	O	PHE	A	400	10.354	27.971	10.616	1.00	23.63
2912	CB	PHE	A	400	12.387	29.922	11.850	1.00	24.14
2913	CG	PHE	A	400	13.306	30.718	12.718	1.00	25.15
2914	CD1	PHE	A	400	13.533	30.424	14.055	1.00	24.96
2915	CD2	PHE	A	400	13.974	31.813	12.170	1.00	25.57
2916	CE1	PHE	A	400	14.385	31.188	14.826	1.00	24.16
2917	CE2	PHE	A	400	14.806	32.600	12.940	1.00	25.43
2918	CZ	PHE	A	400	15.018	32.276	14.270	1.00	25.18

**FIG. 2-47A**

2919	N	GLY	A	401	9.099	29.086	12.115	1.00	24.50
2920	CA	GLY	A	401	7.842	28.848	11.405	1.00	23.46
2921	C	GLY	A	401	7.129	27.661	12.040	1.00	23.34
2922	O	GLY	A	401	6.228	27.052	11.467	1.00	22.92
2923	N	GLY	A	402	7.634	27.221	13.198	1.00	23.63
2924	CA	GLY	A	402	7.103	26.072	13.900	1.00	23.42
2925	C	GLY	A	402	7.077	24.803	13.068	1.00	24.44
2926	O	GLY	A	402	6.208	23.954	13.285	1.00	24.84
2927	N	THR	A	403	8.060	24.585	12.203	1.00	24.96
2928	CA	THR	A	403	8.122	23.374	11.385	1.00	25.60
2929	C	THR	A	403	8.923	22.313	12.123	1.00	25.97
2930	O	THR	A	403	10.091	22.525	12.445	1.00	26.03
2931	CB	THR	A	403	8.711	23.664	10.000	1.00	26.33
2932	OG1	THR	A	403	8.834	22.465	9.225	1.00	26.55
2933	CG2	THR	A	403	10.078	24.329	10.102	1.00	26.08
2934	N	ASN	A	404	8.267	21.206	12.481	1.00	26.32
2935	CA	ASN	A	404	8.883	20.161	13.278	1.00	25.93
2936	C	ASN	A	404	9.004	18.827	12.553	1.00	26.08
2937	O	ASN	A	404	8.216	18.461	11.678	1.00	25.83
2938	CB	ASN	A	404	8.105	19.908	14.575	1.00	26.10
2939	CG	ASN	A	404	7.872	21.156	15.387	1.00	27.31
2940	OD1	ASN	A	404	8.801	21.721	15.968	1.00	27.66

**FIG. 2-47B**



[illegible]

**FIG. 2-47C**

2962	C	ILE	A	408	14.199	5.975	13.852	1.00	32.25
2963	O	ILE	A	408	13.896	5.536	12.746	1.00	31.08
2964	CB	ILE	A	408	12.025	6.322	15.033	1.00	30.12
2965	CG1	ILE	A	408	11.353	7.157	16.132	1.00	29.79
2966	CG2	ILE	A	408	12.305	4.920	15.557	1.00	29.58
2967	CD1	ILE	A	408	9.895	6.798	16.326	1.00	29.42
2968	N	PHE	A	409	15.284	5.614	14.523	1.00	34.35
2969	CA	PHE	A	409	16.214	4.642	13.950	1.00	36.66
2970	C	PHE	A	409	16.134	3.342	14.724	1.00	38.51
2971	O	PHE	A	409	15.690	3.343	15.874	1.00	38.95
2972	CB	PHE	A	409	17.635	5.215	13.925	1.00	36.47
2973	CG	PHE	A	409	17.789	6.215	12.808	1.00	36.23
2974	CD1	PHE	A	409	17.643	7.567	13.065	1.00	36.49
2975	CD2	PHE	A	409	17.991	5.788	11.505	1.00	35.84
2976	CE1	PHE	A	409	17.755	8.487	12.036	1.00	36.42
2977	CE2	PHE	A	409	18.093	6.696	10.475	1.00	36.01
2978	CZ	PHE	A	409	17.977	8.051	10.745	1.00	36.45
2979	N	LYS	A	410	16.465	2.241	14.066	1.00	40.81
2980	CA	LYS	A	410	16.395	0.937	14.720	1.00	42.76

**FIG. 2-48A**

2981	C	LVS	A	410	17.648	0.123	14.412	1.00	43.74
2982	O	LVS	A	410	18.141	0.139	13.281	1.00	42.97
2983	CB	LVS	A	410	15.147	0.184	14.279	1.00	43.67
2984	CG	LVS	A	410	15.072	-1.261	14.749	1.00	45.15
2985	CD	LVS	A	410	13.842	-1.944	14.178	1.00	46.70
2986	CE	LVS	A	410	13.728	-3.393	14.600	1.00	47.69
2987	NZ	LVS	A	410	13.392	-3.506	16.051	1.00	48.43
2988	N	LVS	A	411	18.133	-0.567	15.439	1.00	45.19
2989	CA	LVS	A	411	19.314	-1.409	15.301	1.00	47.01
2990	C	LVS	A	411	18.931	-2.679	14.539	1.00	48.00
2991	O	LVS	A	411	17.858	-3.221	14.794	1.00	47.64
2992	CB	LVS	A	411	19.882	-1.782	16.661	1.00	47.51
2993	CG	LVS	A	411	21.236	-2.461	16.610	1.00	48.43
2994	CD	LVS	A	411	21.829	-2.606	18.008	1.00	49.25
2995	CE	LVS	A	411	21.660	-4.036	18.505	1.00	49.84
2996	NZ	LVS	A	411	22.313	-4.225	19.835	1.00	50.37
2997	N	ILE	A	412	19.767	-3.087	13.601	1.00	49.72
2998	CA	ILE	A	412	19.469	-4.274	12.799	1.00	51.86
2999	C	ILE	A	412	20.459	-5.392	13.085	1.00	52.16
3000	O	ILE	A	412	20.167	-6.540	12.754	1.00	52.95
3001	CB	ILE	A	412	19.422	-3.917	11.307	1.00	53.06
3002	CG1	ILE	A	412	18.129	-4.459	10.671	1.00	53.46
3003	CG2	ILE	A	412	20.640	-4.413	10.543	1.00	53.46
3004	CD1	ILE	A	412	17.892	-3.896	9.278	1.00	53.36
3005	OXT	ILE	A	412	21.521	-5.114	13.639	1.00	52.95

**FIG. 2-48B**

[illegible]

**FIG. 2-48C**

3025	O	HOH	503	26.523	32.326	19.940	1.00	34.45	O
3026	O	HOH	504	28.449	30.874	3.017	1.00	33.79	O
3027	O	HOH	505	24.668	28.038	4.445	1.00	18.32	O
3028	O	HOH	507	15.042	27.512	5.199	1.00	17.31	O
3029	O	HOH	508	29.925	26.579	22.947	1.00	40.78	O
3030	O	HOH	511	23.439	42.041	15.173	1.00	71.80	O
3031	O	HOH	512	22.342	38.099	20.418	1.00	32.70	O
3032	O	HOH	516	10.030	4.324	6.316	1.00	46.02	O
3033	O	HOH	520	13.286	7.231	-11.806	1.00	52.47	O
3034	O	HOH	600	4.344	28.171	14.312	1.00	34.33	O
3035	O	HOH	601	8.984	29.158	15.330	1.00	19.89	O
3036	O	HOH	602	23.826	20.969	14.788	1.00	27.55	O
3037	O	HOH	604	35.933	26.827	5.038	1.00	38.80	O
3038	O	HOH	605	32.286	37.853	-6.692	1.00	46.37	O
3039	O	HOH	606	3.089	3.720	8.561	1.00	61.24	O
3040	O	HOH	607	16.239	-0.824	25.960	1.00	37.31	O
3041	O	HOH	608	6.142	22.763	19.648	1.00	44.37	O
3042	O	HOH	609	6.225	28.059	17.075	1.00	32.61	O

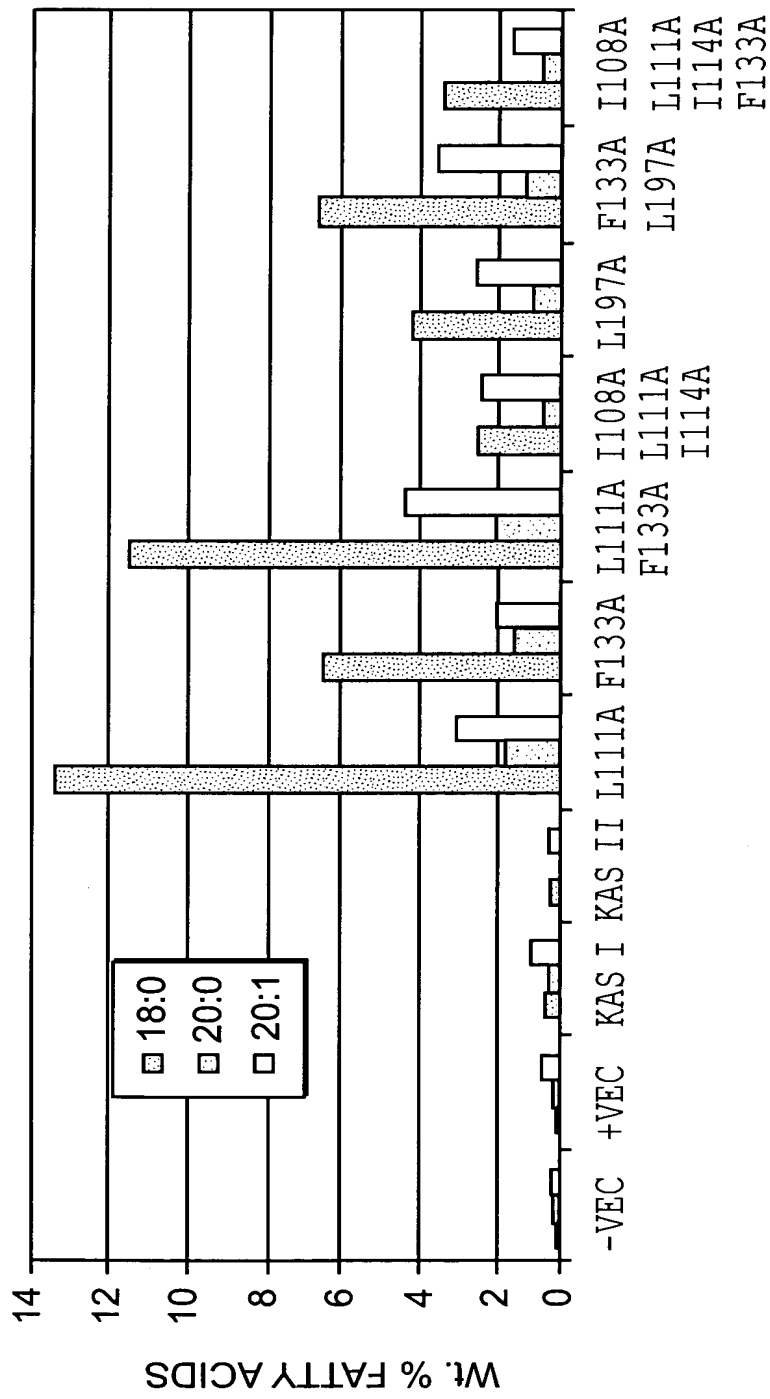
**FIG. 2-49A**

3043	O	HOH	611	32.315	7.695	30.119	1.00	51.98	O
3044	O	HOH	612	32.210	7.634	6.284	1.00	35.28	O
3045	O	HOH	613	17.070	38.017	12.044	1.00	22.73	O
3046	O	HOH	614	31.176	19.825	30.843	1.00	37.36	O
3047	O	HOH	615	27.957	31.368	17.445	1.00	32.76	O
3048	O	HOH	616	32.966	30.345	-2.158	1.00	56.05	O
3049	O	HOH	618	11.323	-4.259	1.793	1.00	38.53	O
3050	O	HOH	620	26.925	5.604	-18.307	1.00	53.90	O
3051	O	HOH	621	16.279	30.145	2.670	1.00	31.13	O
3052	O	HOH	622	38.595	8.716	10.273	1.00	46.13	O
3053	O	HOH	623	33.582	26.804	8.900	1.00	21.60	O
3054	O	HOH	624	21.151	45.870	-3.906	1.00	28.41	O
3055	O	HOH	625	23.504	29.447	25.903	1.00	17.43	O
3056	O	HOH	626	26.368	1.855	-19.938	1.00	44.00	O
3057	O	HOH	627	2.152	6.256	9.459	1.00	47.04	O
3058	O	HOH	628	6.809	19.529	9.383	1.00	29.11	O

**FIG. 2-49B**

3059	O	HOH	629	15.379	11.563	30.794	1.00	48.45	O
3060	O	HOH	630	27.712	4.338	-20.522	1.00	45.95	O
3061	O	HOH	631	18.721	20.451	10.277	1.00	22.11	O
3062	O	HOH	632	31.228	24.084	23.545	1.00	32.43	O
3063	O	HOH	634	39.583	12.746	19.869	1.00	49.30	O
3064	O	HOH	635	25.064	38.355	18.750	1.00	31.27	O
3065	O	HOH	636	28.974	33.743	-7.396	1.00	25.15	O
3066	O	HOH	637	26.250	41.318	16.894	1.00	47.65	O
3067	O	HOH	638	11.568	27.419	17.240	1.00	50.15	O
3068	O	HOH	639	18.706	-6.969	8.775	1.00	47.69	O
3069	O	HOH	640	19.374	-8.885	10.540	1.00	90.15	O
3070	O	HOH	641	22.107	-2.476	12.466	1.00	58.99	O
3071	O	HOH	642	31.157	0.866	24.564	1.00	73.54	O
3072	O	HOH	643	11.493	22.417	31.837	1.00	62.07	O
3073	O	HOH	644	20.933	16.056	-12.243	1.00	35.36	O
3074	O	HOH	645	15.004	40.860	22.656	1.00	47.29	O
3075	O	HOH	646	16.452	-8.745	9.506	1.00	93.19	O

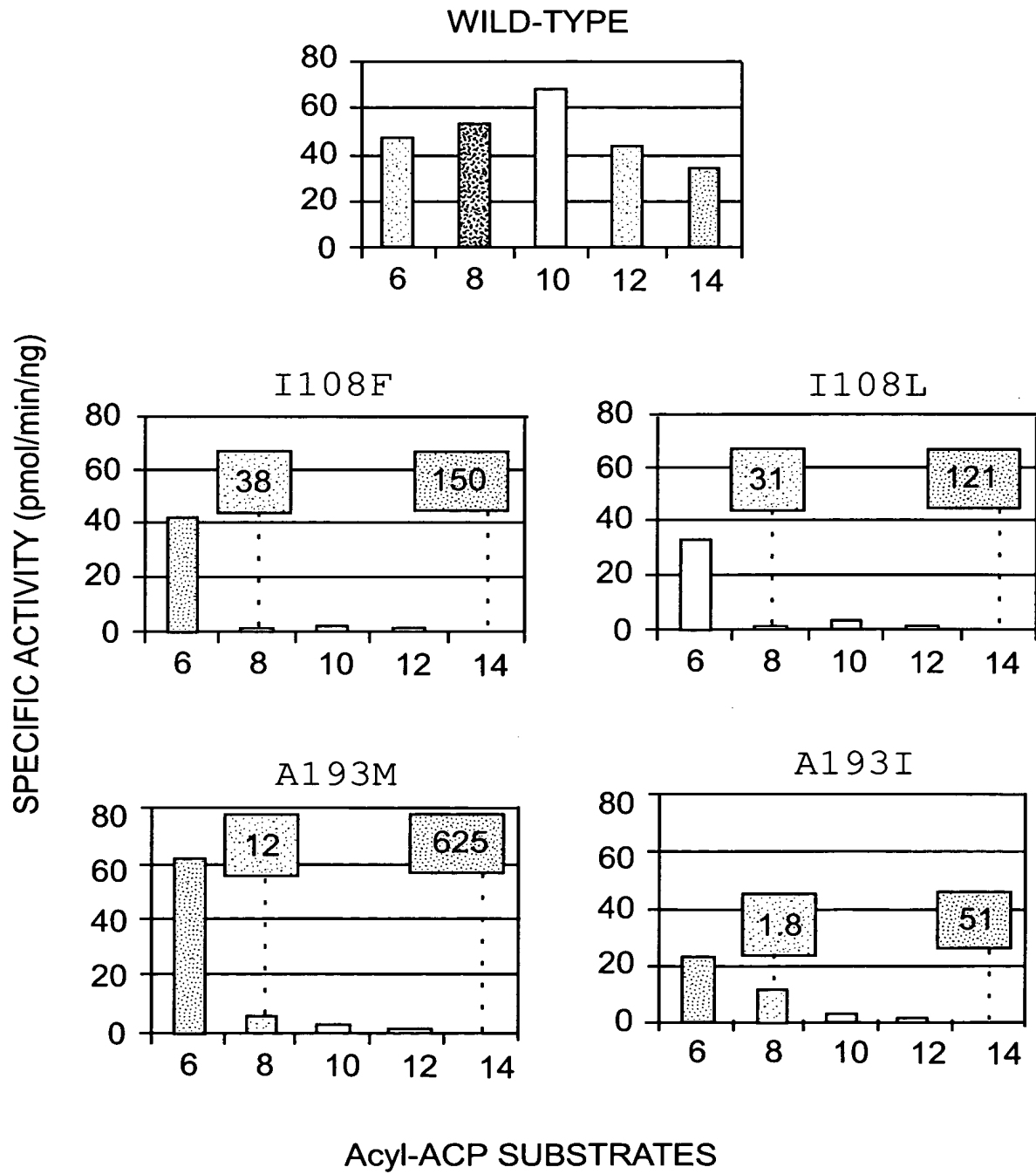
**FIG. 2-49C**



# FIG. 3

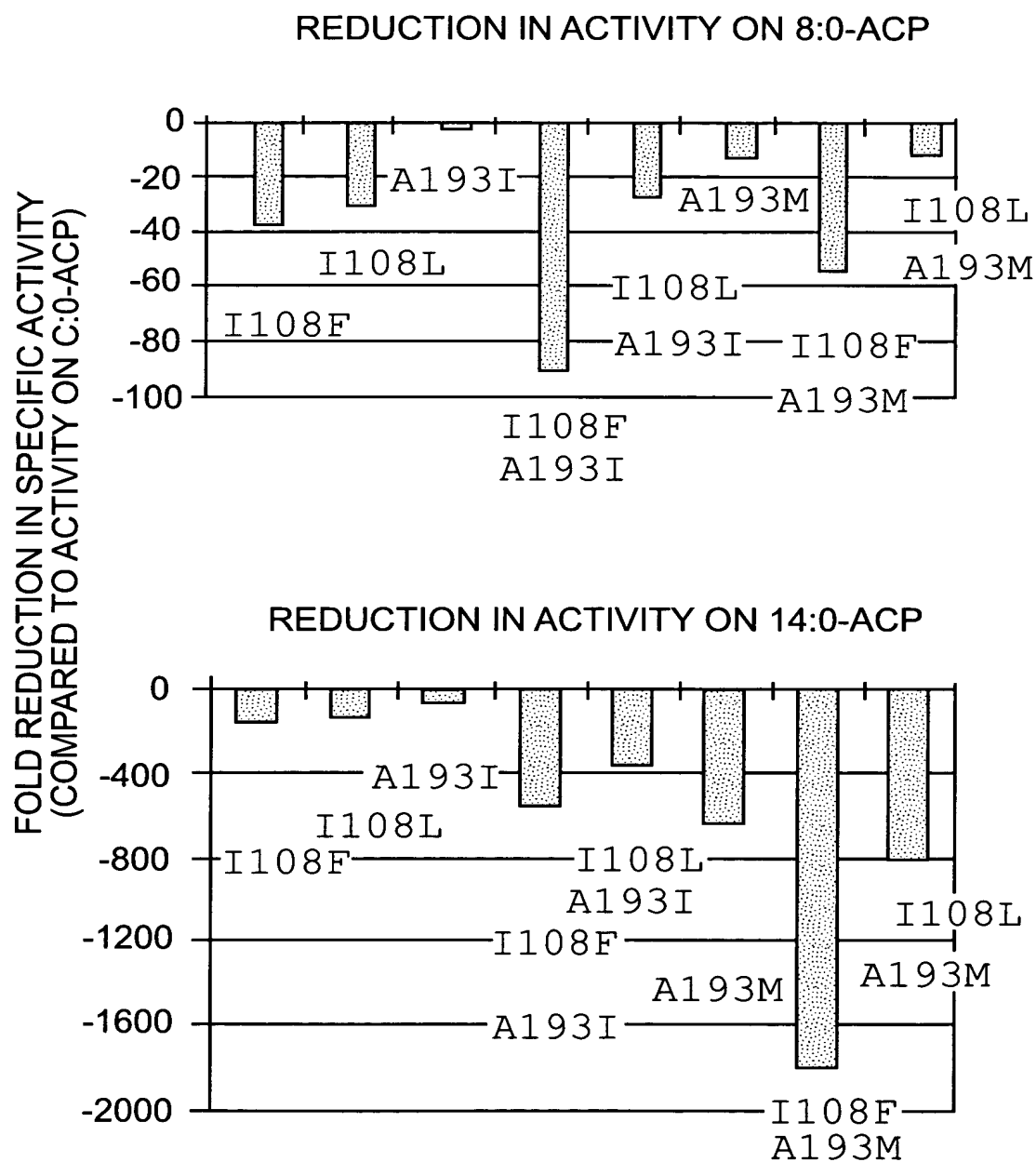


## KAS ASSAY RESULTS



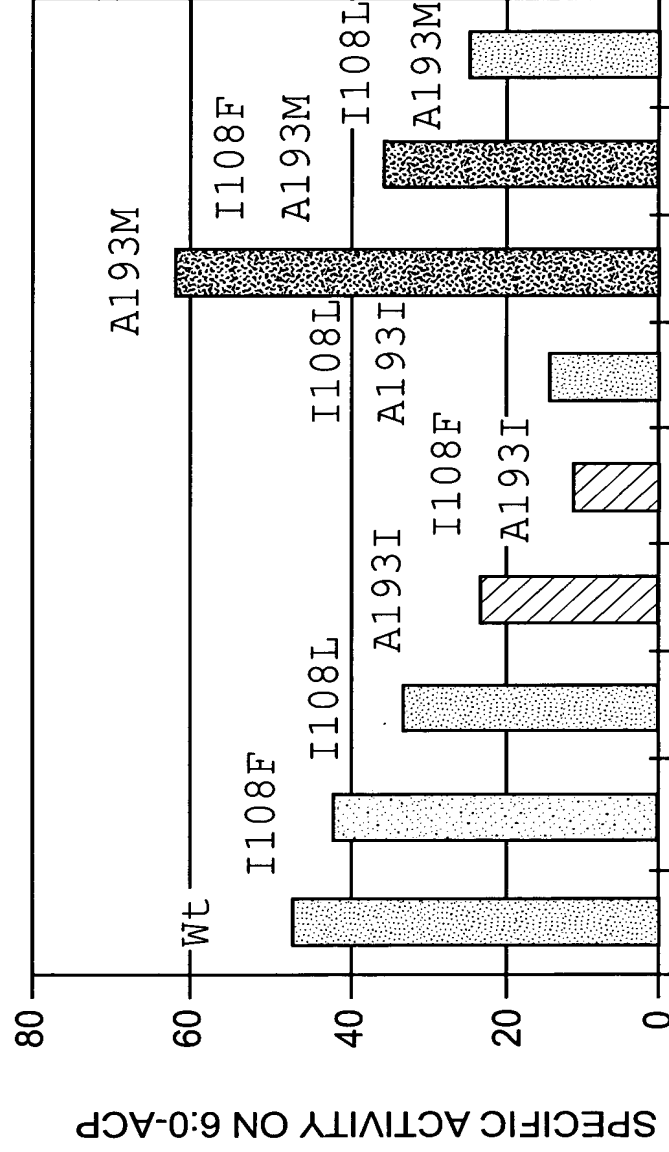
**FIG. 4**

COMPARISON OF THE DECREASE IN ACTIVITY  
ON 8:0 AND 14:0 COMPARED TO 6:0-ACP



**FIG. 5**

COMPARISON OF THE 6:0 ACTIVITY OF THE  
SINGLE AND DOUBLE MUTANTS



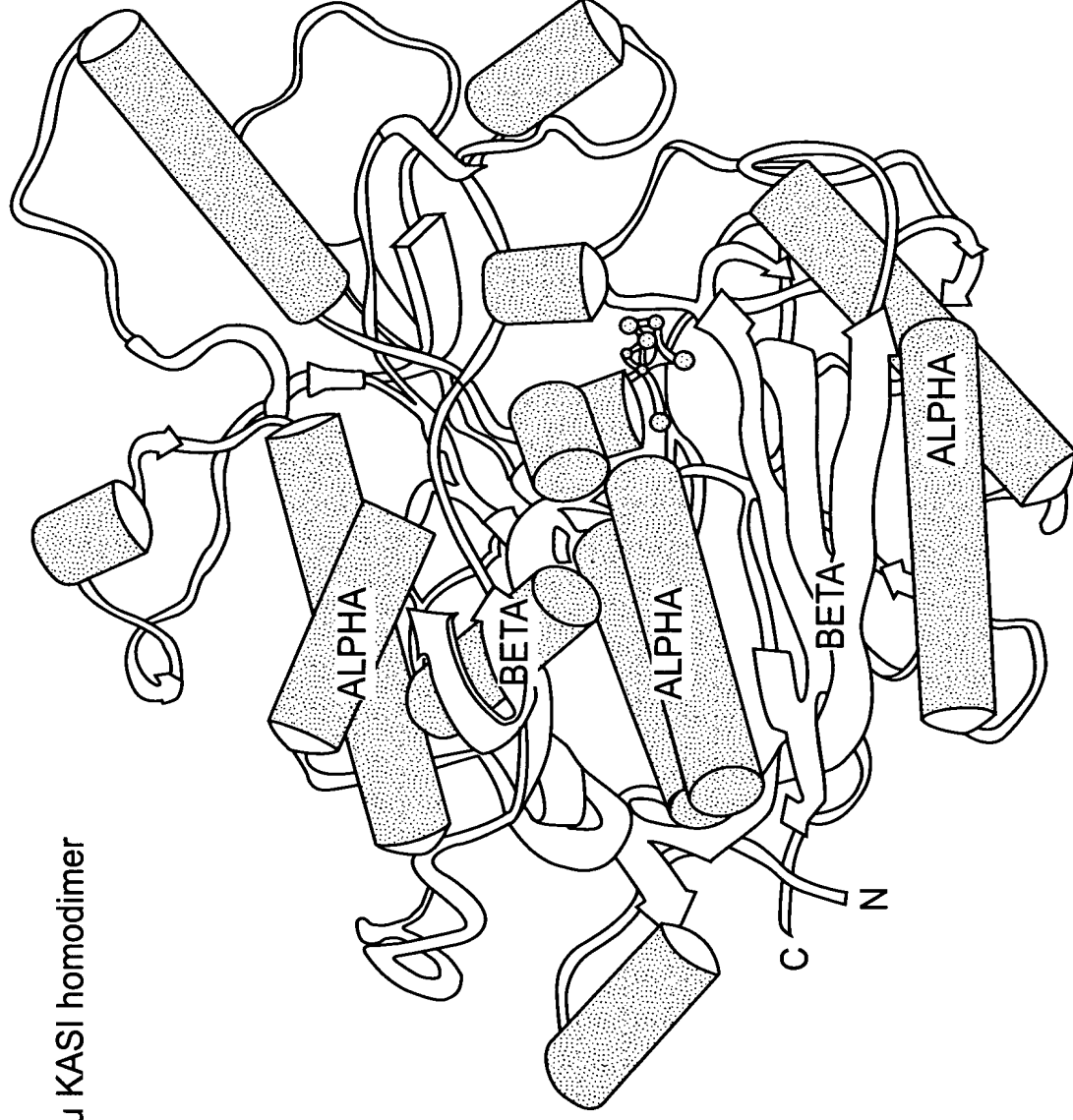
**FIG. 6**

DECREASING THE LENGTH	INCREASING THE LENGTH
I108F	I111A
I108L	F133A
A193I	L111A, F133A
A193M	I108A, L111A, I114A
I108F, A193I	L197A
I108F, A193M	F133A, L197A
I108L, A193I	I108A, L111A, I114A, F133A, L197A
I108L, A193M	

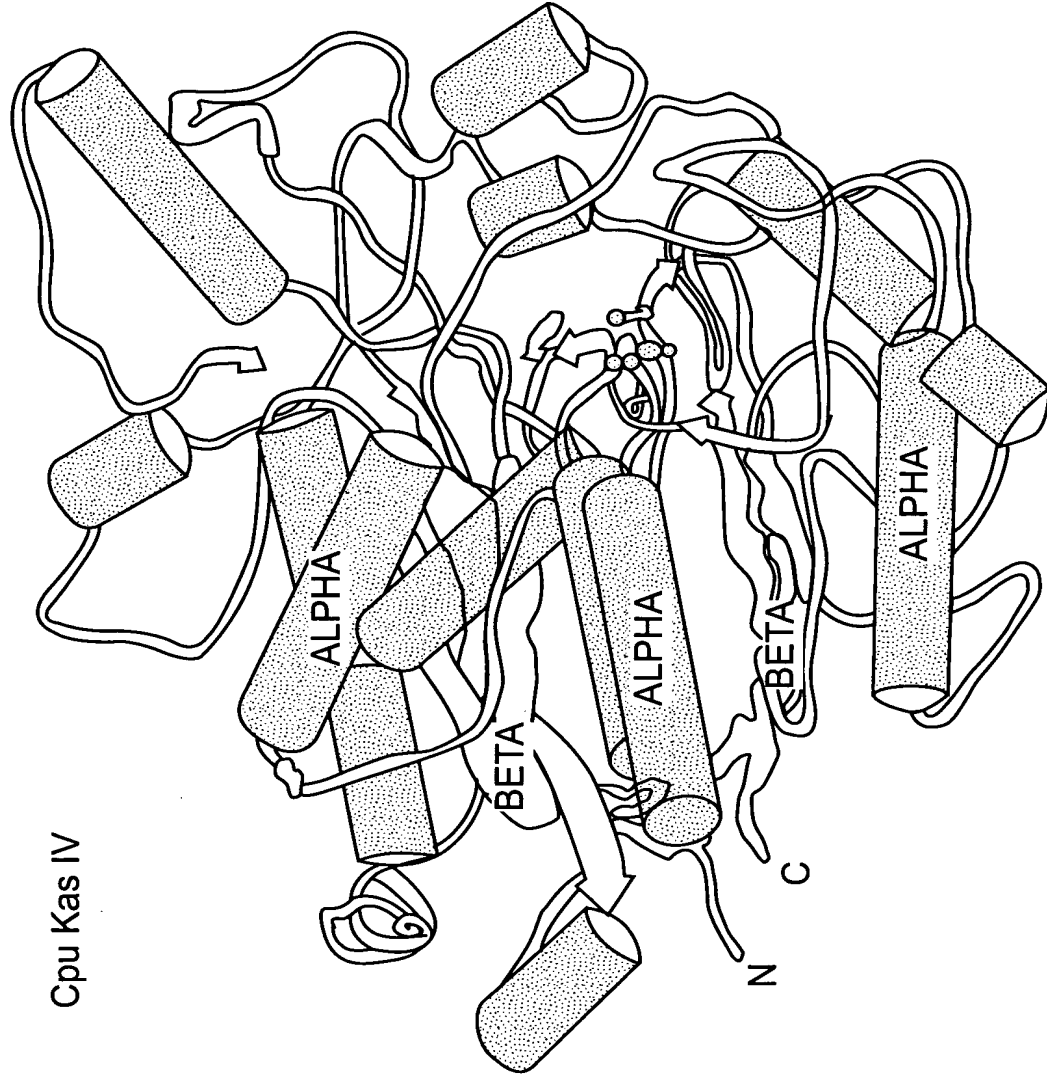
MUTATIONS INTRODUCED INTO E.COLI/KAS II

**FIG. 7**

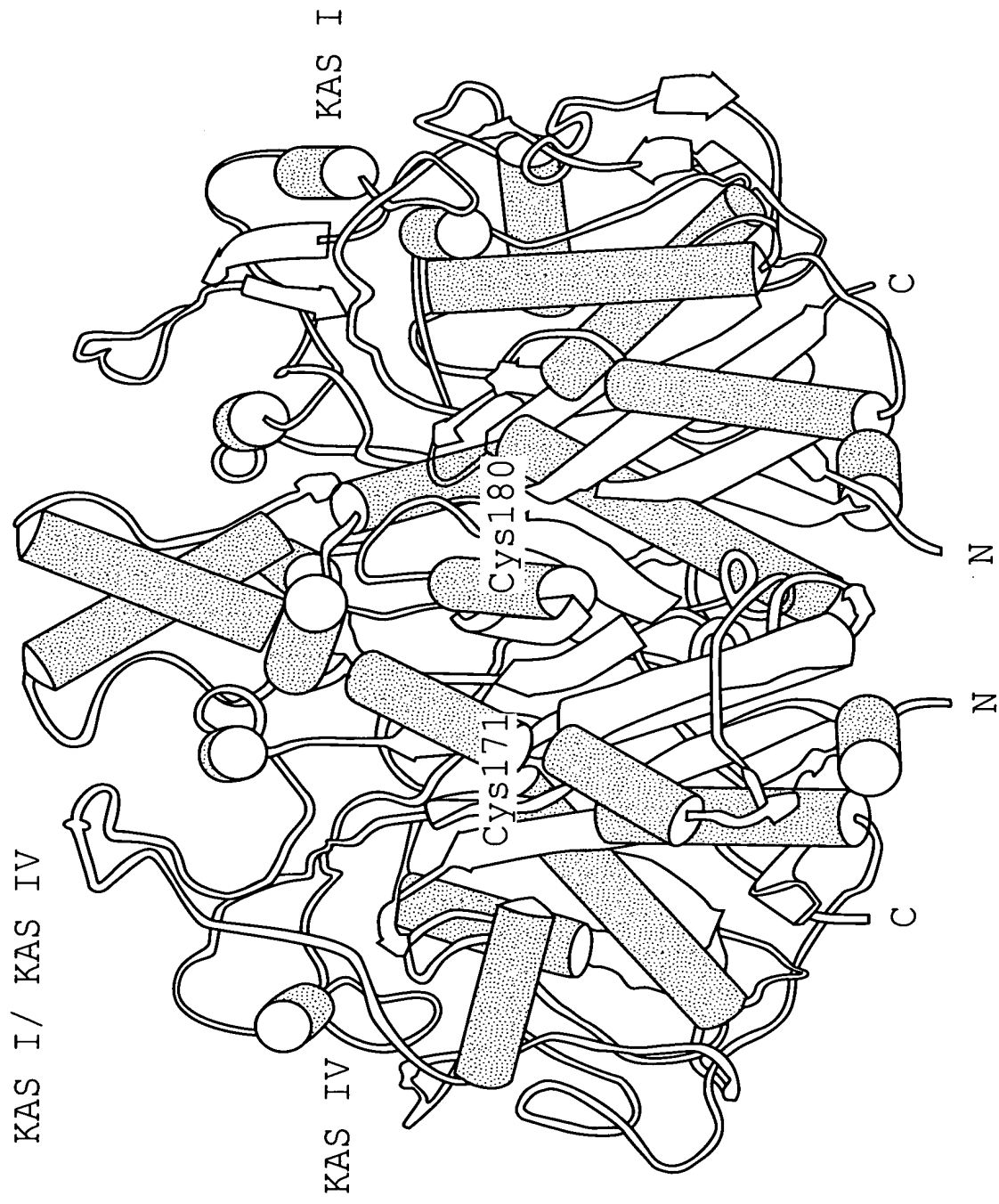
Cpu KASl homodimer



**FIG. 8**



**FIG. 9**



**FIG. 10**

<i>E. COLI</i> KAS II	<i>C. PU</i> KAS IV
I108	M110
L111	M113
L113	V115
I114	F116
F133	C134
I138	T139
L197	I198
G203	V204

SEQUENCE DIFFERENCES  
IN THE HYDROPHOBIC  
POCKETS OF *E. COLI* KASII  
AND *C. PU* KAS IV

**FIG. 11**



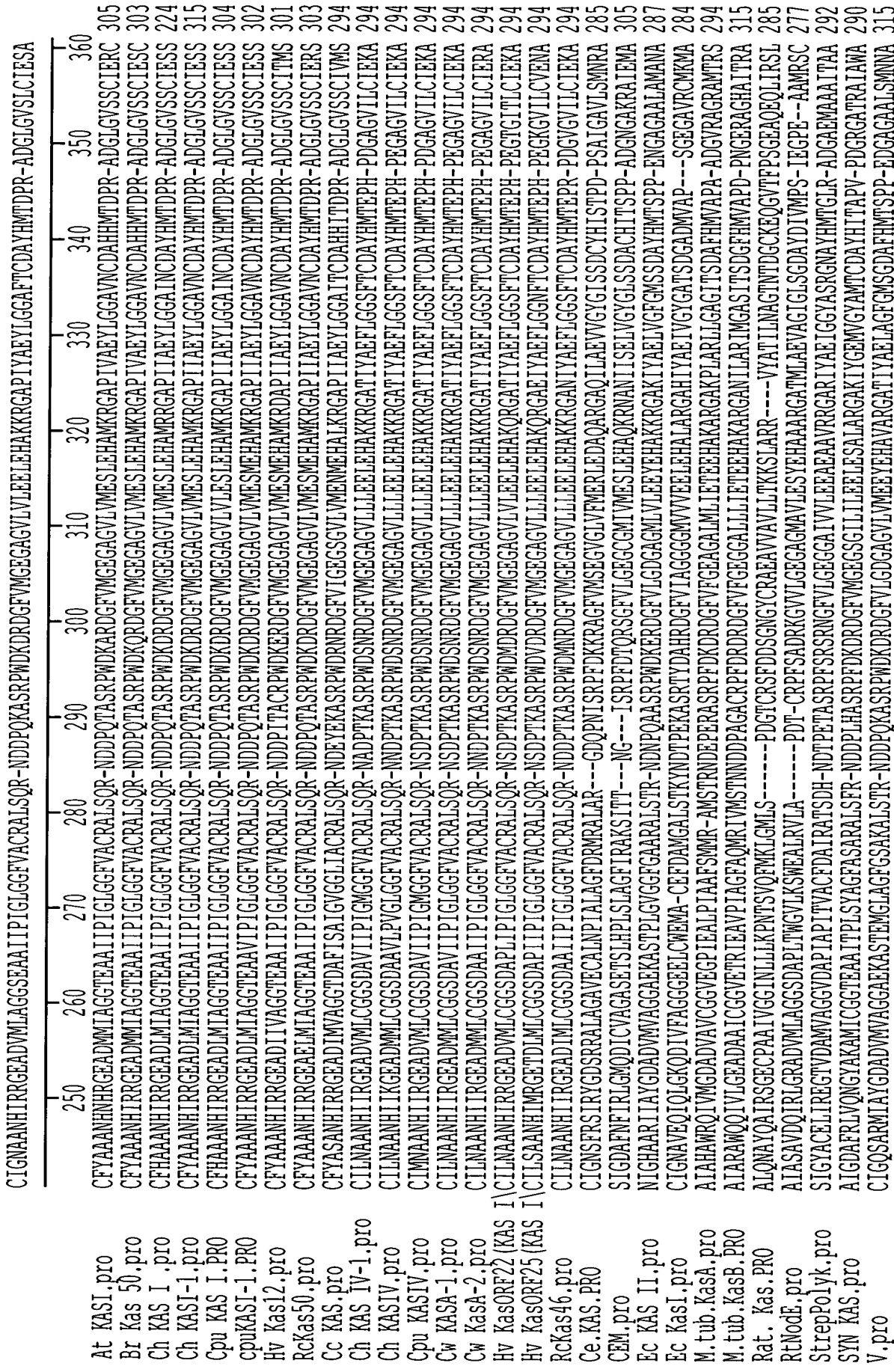
	10	20	30	40	50	60	70	80	90	100	110	120
-K-----	A-K	RRVITGMGVSPGLGHDDVDFYNNLLSGESGISLDR	-----	FDASKFPTRIAEIKS	-----	FSTDGY-IDPK						
At KAS1.pro	IS-----	A-----	SASTVSAPKRETDPK--	KRVVITGMGLVSVCGNDVDAYYEKLLSGESGISLDR	-----	FDASKFPTRFGQIRG	-----	FSSEGY-IDGK	81			
Br Kas 50.pro	-----	A-----	SSSAVSAPKRETKPK--	KRVVITGMGLVSVFGNDVDAYYEKLLSGESGISLDR	-----	FDASKFPTRFGQIRG	-----	FSSEGY-IDGK	79			
Ch KAS I .pro	-----	-----	SSTAVAAALELVDPCCRN	SARA-----	-----	-----	-----	-----	24			
Ch KAS1-1.pro	KL-----	TLTKGNKS-----	WSSTXVAAALELVDPCCRN	SARAGMLVSVFGSDVSVYEKLLSGESGISLDR	-----	FDASKFPTRFGQIRG	-----	FNATGY-IDGK	91			
Cpu KAS I.PRO	RA-----	A-----	SPTVSAPKRETDPK--	KRVVITGMGLVSVFGSDVDAYYDKLLSGESGIGPIDR	-----	FDASKFPTRFGQIRG	-----	FNSMGY-IDGK	80			
cpuKAS1-1.PRO	RA-----	A-----	TASAPKRESDPK--	KRVVITGMGLVSVFGSDVDAYYDKLLSGESGISLDR	-----	FDASKFPTRFAGQIRG	-----	FNATGY-IDGK	78			
Hv Kas12.pro	-----	-----	TSAAPQRETDPK--	KRVVITGMGLASVFGSDVTFYDRLLAGESGVPIDR	-----	FDASSFPTRFAGQIRG	-----	FSSEGY-IDGK	75			
RcKas50.pro	NN-----	-----	NTTISAPKREKOPR--	KRVVITGTGLVSVFGNDVDYDKLLAGESGIGLIDR	-----	FDASKFPTRFGQIRG	-----	FNSQGY-IDGK	79			
Cc KAS.pro	-----	-----	KRETDPK-----	KRVVITGMGLVSVFGSDIDNFYNNKLLGCGSGISLDR	-----	FDASSYTBRAFQIRD	-----	FSSEGY-IDGK	70			
Ch KAS IV-1.pro	KK-----	K-----	PSIKQ-----	RRVVVTGMGVWTPGLCHDPDVFYNNLLDGTSGISEIET	-----	FDCAQFPTRIAEIKS	-----	FSTDGW-VAPK	71			
Ch KASIV.pro	NK-----	K-----	PATKQ-----	RRVVVTGMGVWTPGLCHDPDVFYNNLLDGTSGISEIEN	-----	FDCSQFPTRIAEIKS	-----	FSTDGW-VAPK	71			
Cpu KASIV.pro	KK-----	K-----	PSIKQ-----	RRVVVTGMGVWTPGLCHDPDVFYNNLLDGTSGISEIET	-----	FDCAQFPTRIAEIKS	-----	FSTDGW-VAPK	71			
Cw KASA-1.pro	KK-----	K-----	PVIKQ-----	RRVVVTGMGVWTPGLCHEPDVFYNNLLDGVSGISEIET	-----	FDCQFPTRIAEIKS	-----	FSTDGW-VAPK	71			
Cw Kasa-2.pro	KK-----	K-----	PVTQK-----	RRVVVTGMGVWTPGLCHDPDVFYNNLLDGVSGISEIET	-----	FDCQFPTRIAEIKS	-----	FSTDGW-VAPK	71			
Hv KasORF22 (KAS I\K	I\KK-----	R-----	PDVKQ-----	RRVVVTGMGVWTPGLCHDPDVFYNNLLDGHSGISEIET	-----	FDCSKFPTRIAEIKS	-----	FSTEGW-VVPK	71			
Hv KasORF25 (KAS I\N	I\NN-----	K-----	SETKQ-----	RRVVVTGMGVWTPGLCHEPDEFYNNLLQGVSGVSEIEA	-----	FDCSSYPTRIAEIKS	-----	FSTDGW-VAPK	71			
RcKas46.pro	NK-----	K-----	PLMKQ-----	RRVVVTGMGVSPGLCHDIDVFYNNLLDGSSGISQIDS	-----	FDCAQFPTRIAEIKS	-----	FSTDGW-VAPK	71			
Ce.KAS.PRO	MK-----	LKINKN-----	FEM-----	HRVVTGMCAISPGVTYNALRNGINEGRSGL-----	-----	KYDEILKFVXGAVPGERVEDRWSTGQOREMSKASMFVLAAS	84					
CEM.pro	MS-----	-----	-----	RRVVTGLGCVTPIGRSLSSESNGNLLSKNGLTPTISLPYNNEDYKLEKSIPSTITVKGIPENFQWENSAINKLLFTSQ	82							
Ec KAS II.pro	-----	-----	MSK-----	RRVVVTGLMLSPVGNVTVESTWKALLAGOSGISLIDH	-----	FDTSAVATKFAGLVKD	-----	FNCEDI-ISRK	66			
Ec KasI.pro	M-----	-----	-----	KRAVITGLGIVSSIGNNQEVLASIREGRSGITFSQE	-----	LKDSGMRSHVWGNVK	-----	LDTTGL-IDRK	63			
M.tub.KasA.pro	MSQP-----	STANGG-----	-----	FPSVWVTAVTATTSPIESTWKGLLAGESGIALED	-----	EFTVKWDIAVKIGCHLK	-----	DPVDSHMGR	75			
M.tub.KasB.PRO	MGVP-----	PLAGASRTDM-----	EGTFARPMTVELVTGKAPPYVVVTGIAMTTALATDAETTKWLLLDQSGIRLDD	-----	PFVEEFDLPVRIGCHLL	-----	EEFDHQLTRI	95				
Rat. Kas.PRO	-----	-----	SRASQRAMEEVIAGMSCKLPESNLOEFWANLIGGVDWVTDDDR	-----	RWKAGL	-----	YGLPKR-SGKLKD	-----	SKFDASFFGVHPK	79		
RtNodeI.pro	MD-----	-----	RRVVTGIGLGLGTNAASINWEMREGFSAISPIIT	-----	TDLYDLEGTVGLEIK	-----	AIP-EHDIPRK	64				
StrepPolyk.pro	VN-----	-----	RRVITGIGVWAPGAVGTPFWELLSCGTATRAIST	-----	FDATPFRSRIAECD	-----	FDPVAAGLSAE	65				
SYN KAS.pro	-----	-----	MANLEK-----	KRVVVTGLCAITPTIGNTLQDYWGMEGNIGIGPITR	-----	FDASDOACRFGEVKD	-----	FDATQF-LDRK	69			
V.pro	SDYHNHF	INVKAVARPLFFCLFWRTSVANN	-----	RRVVTGIGIVSPVGNVTATATAWEAIKSGISGIEIENIEH	-----	FDTTNTSTKFAGLVND	-----	FDAESVGINRK	94			

FIG.12-1

NSRRMDDFMRYCIVAGKKALEDAGLGE--D-LSEL---DKERAGVLIG-SGMGGLKVFSDGVQVLEAL-EKG-----YRKISPFVPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY  
 130 140 150 160 170 180 190 200 210 220 230 240  
 NERRLDDCLRYCIVAGKKALESANLGG--DKLNTI---DKRKAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRRISPPFIPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY 187  
 NERRLDDCLRYCIVAGKKALESANLGG--DKLNTI---DKQKAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRRISPPFIPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY 185  
 -----DIGA--DRLSKI---DKERAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRKITPFFIPVPAITNMGSALLAIEFGLMGNPNSISTACATSNY 106  
 NDRRLDDCLRYCIVAGKKALENSDLGG--ESLSKI---DKERAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRRISPPFIPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY 197  
 NDRRLDDCLRYCIVAGKKALEDADLGA--DRLSKI---DKERAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRKITPFFIPVPAITNMGSALLAIEFGLMGNPNSISTACATSNY 186  
 NDRRLDDCLRYCIVAGKKALEDADLAG--QSLSKI---DKERAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRRISPPFIPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY 184  
 NDRRLDDCLRYCIVAGKKALEDADLHKL---DVCRAGVLVG-TGMGGITVFESEGVQVNLIEKG-----YRKISPPFIPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY 183  
 NDRRLDDCLRYCIVAGKKALEDADLGG--DKLSKI---DKERAGVLVG-TGMGGITVFESEGVQVNLIEKG-----HRKITPFFIPVPAITNMGSALLAIEFGLMGNPNSISTACATSNY 185  
 NDRRLDDCLRYCIVAGKKALEDANLGG--QVLDTM---DKTRIGVLVG-SSMGSKVFADAVEALVQRG-----YKINPFFIPVPAITNMGSALLAIDLGLMGNPNSISTACATSNY 176  
 LSKRMDKFMVLYLTAGKKALENGGITE--DVMKEL---DKRKCVLIG-SAMGGWKVFNDALIEAL-RIS-----YKKNPFCVFPATTNMGSAMLMDLGMGNPNSISTACATSNF 176  
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 LSKRMDKFMVLYLTAGKKALENGGITE--EVMKEL---DKRKCVLIG-SAMGGWKVFNDALIEAL-RIS-----YKKNPFCVFPATTNMGSAMLMDLGMGNPNSISTACATSNF 176  
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 LSKRMDKFMVLYLTAGKKALENGGITE--EVRNEL---DKTRCVLIG-SAMGGWKVFNDALIEAL-RIS-----YKKNPFCVFPATTNMGSAMLMDLGMGNPNSISTACATSNF 176  
 LSKRMDKFMVLYLTAGKKALENGGITE--DIMNEL---DKSRCVLIG-SAMGGWKVFNDALIEAL-RIS-----YKKNPFCVFPATTNMGSAMLMDLGMGNPNSISTACATSNF 176  
 LSKRMDKFMVLYLTAGKKALENGGITE--DMMDEL---DKARCVLIG-SAMGGWKVFNDALIEAL-RIS-----YKKNPFCVFPATTNMGSAMLMDLGMGNPNSISTACATSNF 176  
 EE-----ALKQKAEVDVHNETLVN-----IGTQMSDLIEH-----IG-ETAQKVSE-----GQS-----RRVSPVFPVPRILNLPAGYVAMKYMRGGVVESTSTACATGLH 169  
 DERRTSSFIKALRTTYEALHNAGLNPNDITNTSLCNLDHFCLLIG-SGIGSIQDIYQTSLOFHNDN-----KRINPFFVPKLTNNAGNVSIKENIRGLSHSVSTACATGN 192  
 EQKRMDAFIQYGVAGVQAMQDSGLE-----ITEE---NATRIGAAIG-SGIGGLGLEENGTSMLMNGG-----PRKISPFVPSTIVNMVAGHLTIMYGLRGPSISIACTSGVH 169  
 VVRFMSDASTIYAFLSMEQALADAGLSPEA---YQ---NNPRVGLIAG-SGGG-----SPRFQVFGADAMRGR--GLKAVGPVVTKAMASGVSACTATPFKIHGVNYSISSACATSAH 168  
 DMRMSYQRMGKLLGGQWESAG-----SPEV---DPDRFAVVG-TGLGAERIVESYDLNMAGGP-----RKVSPVAVQIMPNGAAAVTGLQIGARAGVWTPVSACSSGE 176  
 ELRNMGYLQRMSTVLSRLWENAG-----SPEV---DTNRLMVSIG-TGLSAAELVFSYDDMRARGM-----KAVSPITVQKYPMPNGAAAVGLERHAKAGVWTPVSACASGAE 196  
 QAHTWDPQLRLLEVSYEALVDGGINPASLR-----GTNTGVWVGVSVSASEALSRDPETLLG-----YSMWCCQRAMNANRISFFFFKFGPSIALDTACSSSL 175  
 QLVSMDFRSLJAVTAATEAMKQAGL-----SCDEQ---NAHRFGAAMG-LGGPWDTTEETYSILLDGVTRARIFTAPKG-----MPSAAAGHVSIFLGLRGVPFGVTSACAAGVH 167  
 QARRLDRAQFALVAGQEALEADSLG-----RIDED---SAHRVGVCVG-TAVGCTQKLESEY--VALSAGGAHWVDPCRGSPELYDFVPSLAAEVAWLGAEGPNIVSAGCTSGLD 174  
 EAKRMDRFCHFVACASQQAINDAKLV-----INEL---NADEIGVLIG-TGIGGKVLVEDQQTILLDKG-----PSRCSFMIPIWMIANNASGLTAINLGAKPNNCTVTACAAGSN 172  
 DCRKMDLFIQYGIAAAEQALTDSGLE-----ITEQ---NATRIGTAIG-SGIGGLGLEQNVHVSFKVG-----ARKVSPFFVPVPAITNMVAGHVSIRNNLKPNIATACTSGTH 197

At KAS I.pro  
 Br Kas 50.pro  
 Ch KAS I .pro  
 Ch KAS I-1.pro  
 Cpu KAS I.PRO  
 cpuKAS I-1.PRO  
 Hv Kas12.pro  
 Rckas50.pro  
 Cc KAS.pro  
 Ch KAS IV-1.pro  
 Ch KAS IV.pro  
 Cpu KAS IV.pro  
 Cw KASA-1.pro  
 Cw Kasa-2.pro  
 Hv KasORF22 (KAS I)  
 Hv KasORF25 (KAS I)  
 Rckas46.pro  
 Ce.KAS.PRO  
 CEM.pro  
 Ec KAS II.pro  
 Ec KasI.pro  
 M.tub.KasA.pro  
 M.tub.KasB.PRO  
 Rat. Kas.PRO  
 RNode.pro  
 StrepPolyk.pro  
 SYN KAS.pro  
 V.pro

**FIG.12-2**



**FIG.12-3**

	LADAGVSPEDVNYINAHATSTPAGDLAEINAIKKVFF---GQNS-ELKVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DPGVLDLLLVGNKK-----EQHEVKVAL	370	380	390	400	410	420	430	440	450	460	470	480
At KAS1.pro	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KSTS-GIKINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EQAVDEDT-VPNEK-----KQHEVDVAI	411											
Br Kas 50.pro	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KSTS-GIKINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPAVDEDT-VANEK-----KQHEVNVAI	409											
Ch KAS I .pro	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KNTK-DIKINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPSVEEDT-VANKK-----QQHEVNVAI	330											
Ch KASI-1.pro	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KNTK-EITINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPSVEEDT-VANKK-----QQHEVNVAI	421											
Cpu KAS I.PRO	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KNTK-DIKINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPSVEEDT-VANKK-----QQHEVNVAI	410											
cpuKASI-1.PRO	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KNTK-EIKINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPSVDENT-VANKK-----QQHEVNVAI	408											
Hv kas12.pro	LRDAGVAPPEVNYINAHATSTLAGDLAEINAIKKVFF---KNPS-EIKNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPEVDEDT-VANEK-----KQHEVNVAI	407											
RcKas50.pro	LEDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KNTS-DIKINATKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPSVEEDT-VANKK-----QQHEVNVAI	409											
Cc KAS .pro	LVDAGVSPPEVNYINAHATSTLAGDLAEINAIKKVFF---KOTS-EIKMNGTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EPQVTIDT-VPNVK-----KQHEVNVAI	400											
Ch KAS IV-1.pro	LAQSGVSREDVNYINAHATSTPAGDIKEIQAALHCF---GQNN-ELKVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DEGVDTKLLVGPCK-----ERLNVKVL	401											
Ch KASIV.pro	LAQSGVSREDVNYINAHATSTPAGDIKEIQAALHCF---GQNS-ELRVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DEGVDAKLLVGPCK-----EKLKVKVGL	401											
Cpu KASIV.pro	LAQSGVSREDVNYINAHATSTPAGDIKEIQAALHCF---GQNR-ELKVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DEGVDTKLLVGPCK-----ERLNVKVL	401											
Cw KASA-1.pro	LAQSGVSKEDVNYINAHATSTPAGDIKEIQAALHCF---GQNS-ELRVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DKAVDAKLLVGPCK-----ERLNVKVL	401											
Cw Kasa-2.pro	LAQSGVSKEDVNYINAHATSTPAGDIKEIQAALHCF---SQNS-ELRVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DDGVDAKLLVGPCK-----EKLKVKVGL	401											
Hv KasORE22 (KAS I)	LADSGVAREEINYNHAHATSTQSGDLKEIQAALHCF---GQNP-QLRVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EKVDVGLVGSSEK-----ERCEVKVAL	401											
Hv KasORE25 (KAS I)	LADAGVTRODINYNHAHATSTQGLKEIQAALHCF---GQNP-QLRVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EKNVDVSLLVGSQK-----ERCDVKVAL	401											
RcKas46.pro	LARSVSKSEEVNYINAHATSTPAGDIKEIQAALHCF---SQNP-DLRVNSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----EEGVDTKVLPCK-----ERLDIKVAL	401											
Ce.KAS.PRO	IGNAHLEPKDIGYNHAHATSTPNGDSVEAEV-RQVFPEQNI A---VSSVKGHIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----ETDEGNGLNLRNQKWSVGNKSRISI	395											
CEM.pro	LKWARLEPTDQVYNHAHATSTLIGDKAECLAVASALLPCRSKSKPLYTSSNKGAIHIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DEGCDIDFVPHEAR-----QVSGMEYTL	421											
Ec KAS II.pro	LRDAGIEASQIGYNHAHATSTPAGDKAEQAQVKTF---GEAASRVLSVSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DEQAA-GLNIVTET-----TDRELTVM	395											
Ec KasI.pro	MHGVDTP---IDYLNSHGTSTPVGDVKELAA IREVF---GDKS--PAISATKAMTGHSLGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DEQAA-GLNIVTET-----TDRELTVM	386											
M.tub.KasA.pro	LELAGLSPADIDHYNHAHATSTPIGDAAEANA IRVA---GCDQ--AAIYAPKSAHGSLGAGGLEAIATVKAIRTGWIHTPTINLENP-----DPEIDLDVAGEPR-----YG-DYRVAV	398											
M.tub.KasB.PRO	IQLAGLPGDIDHYNHAHATSTQVGLAEGRA INNAL---GGNR--PAYAPKSAHGSLGAGGLEAIATVKAIRTGWIHTPTINLENP-----DPEIDLDVAGEPR-----PG-NYRVAI	420											
Rat. Kas.PRO	YQPGVAPESLEYTEAHGTGTVGPQOELNGITRSLCAFRQSP---LLJGSTKSNMGHPEPASGLAALTKVLLSLENGWAPNLHFNHP-NPEIPALLDGLQVDRP---LPVRGGIVGI	399											
RNode.pro	LADAEINPDVDYINAHATSTVANDEMETA IIRVF---GDHAFQMSVSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DQCDLDVTPNVPR-----EQR-C-GSM	383											
StrepPolyk.pro	LDEARRDPSVDYINAHATSTKQNDRHETSAFRSL---GEHAVRPVSSIKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DPEIDLDVYVLTAR-----EKR-VRHAL	399											
SYN KAS.pro	LKDSGLKPEWVSYINAHATSTPANDVTEIRA IKAAL---GNHAYINAVSSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----DPECIDLDYVPGQSR-----ALI-VDVAL	397											
V.pro	IADAGITADKVGYNHAHATSTPAGDKAEIQAALHCF---GEHAYTLAVSSTKSMIGHLILGAAGGLEAIATVKAIRTGWIHTPTINLENP-----SEGCDLDYVTDGAR-----PYN-METAL	422											

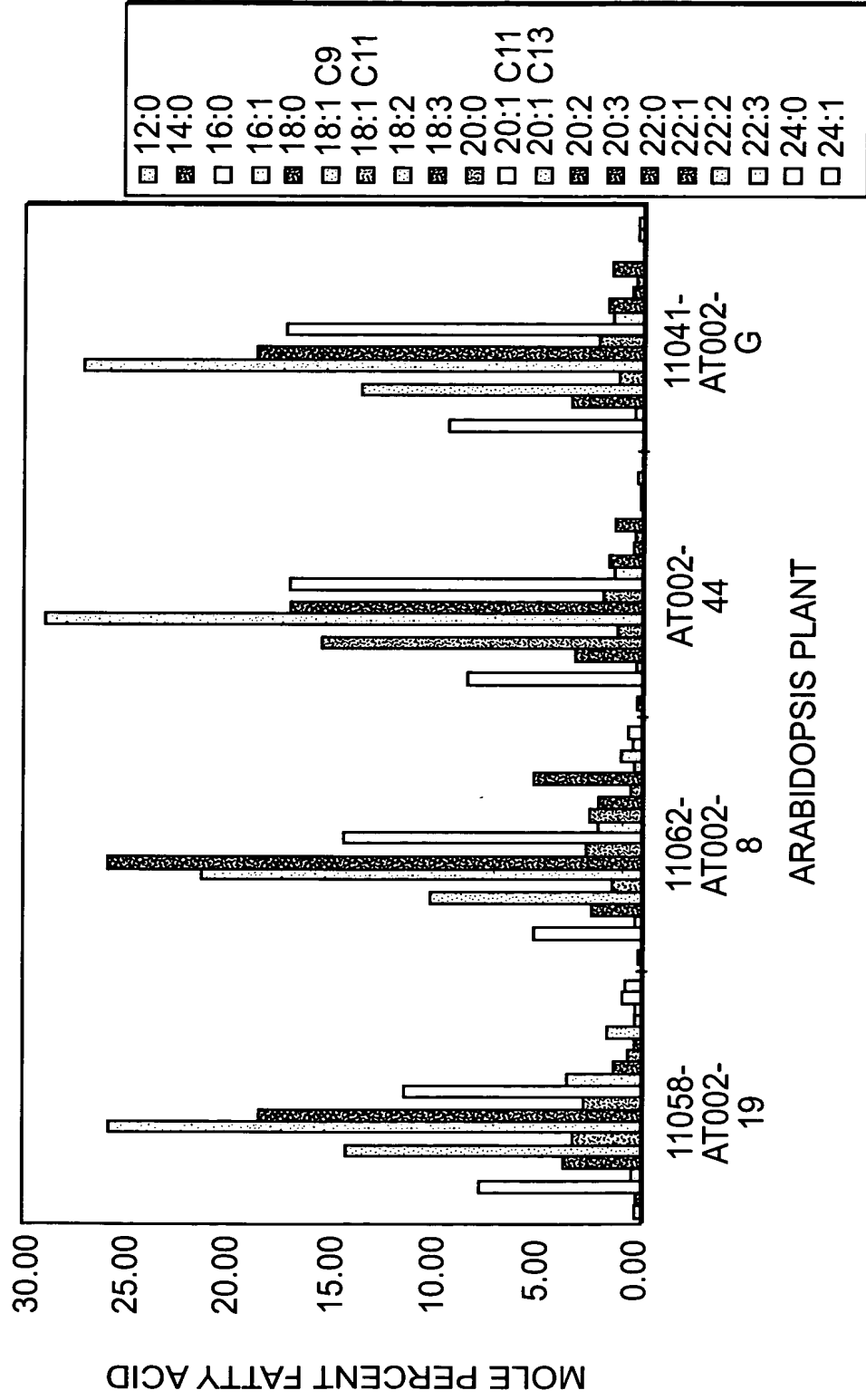
**FIG.12-4**

SNSFGFGGHNSSVAFAPFK--  
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 490 500  
 At KASI.pro SNSFGFGGHNSSVAFSAFK-P  
 Br Kas 50.pro SNSFGFGGHNSSVAFSAFK-P  
 Ch KAS I .pro SNSFGFGGHNSSVAFSAFK-P  
 Ch KASI-1.pro SNSFGFGGHNSSVAFSAFK-P  
 Cpu KAS I.PRO SNSFGFGGHNSSVAFSAFK-P  
 cpuKASI-1.PRO SNSFGFGGHNSSVAFSAFK-P  
 Hv Kas12.pro SNSFGFGGHNSSVAFAPFK-P  
 RkKas50.pro SNSFGFGGHNSSVAFSAFK  
 Cc KAS.pro SNSFGFGGHNSSVAFAPYK-P  
 Ch KAS IV-1.pro SNSFGFGGHNSSILFAPY--N  
 Ch KASIV.pro SNSFGFGGHNSSILFAPCN  
 Cpu KASIV.pro SNSFGFGGHNSSILFAPY--I  
 Cw KASA-1.pro SNSFGFGGHNSSILFAPCN-V  
 Cw Kasa-2.pro SNSFGFGGHNSSILFAPCN  
 Hv KasORF22(KAS I\SNSFGFGGHNSSILFAPFK  
 Hv KasORF25(KAS I\SNSFGFGGHNSSILFAPF  
 RkKas46.pro SNSFGFGGHNSSILFAPYK  
 Ce.KAS.PRO CNSFGFGATNASLILKQF  
 CEM.pro CNSFGFGGVNTSLLEFKWEGS  
 Ec KAS II.pro CNSFGFGGTNGSLIF  
 Ec Kasi.pro SNSFGFGGTNATLVNRKLIK-D  
 M.tub.KasA.pro NNSFGFGGHNVALAFGRY  
 M.tub.KasB.PRO NNSFGFGGHNVAIAFGRY  
 Rat. Kas.PRO -NNSFGFGGANVHVILQP-NAS  
 RtNode.pro SNAFAMGGTNAVLAFRQV  
 StrepPolyk.pro TVSGFGGFGQSAMLLSRLE-R  
 SYN KAS.pro SNSFGFGGHNVTIAFKKYQ  
 V.pro SNSFGFGGTNGSLLEFKKAD

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FIG.12-5

# FATTY ACID COMPOSITION OF T2 POOLED SEED



**FIG. 13**

**Bgl II site SalI site**

CTG**AGATCTGTCGACAT**GCGGACCGCTTCTCGCATGGTTGCGTCCCCTTTCTGTACGTGGC  
TCGTAGCTGCATGCCCCACTTCAATCCGACAACGACCCACGTTCCCTTTCCCAACAAGCGGCT  
CCGCCCTCTCCCGTCGCGGAGGACTCTCTCTCCCATTTGCTCCCTCCGCGGATCCACCTTCCAA  
TGCCTCGATCCTTGCAACCAAGCAACGCTTCTCGGGGATAACGGATTGCTTCCCTCTTCGGAT  
CCAAGCCTCTTCGTTCAAATCGCGGCCACCTGAGGCTCGGCCGCACTTCCCATTCGGGGAGG  
TCATGGCTGTGGCTATGCAACCTGCACAGGAAGTCTCCACA**AGATCT**GTC

**Bgl II site**

**FIG.14**